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VOLUME 9

STUDY TITLE

Summary of the OPPTS 870 Series Human Health Data Requirements:
Capric Acid (Decanoic Acid)

DATA REQUIREMENTS

OPPTS Test Guidelines: 870.1100 – 870.5375

COMPLETION DATE

March 28, 2013

COMPILED BY

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STUDY ID

Not Applicable

STATEMENT OF NO DATA CONFIDENTIALITY CLAIMS

No claim of confidentiality, on any basis whatsoever, is made for any information contained in this document. I acknowledge that information not designated as within the scope of FIFRA § 10(d)(1)(A), (B) or (C) and which pertains to a registered or previously registered pesticide is not entitled to confidential treatment and may be released to the public, subject to the provisions regarding disclosure to multinational entities under FIFRA § 10(g).

Company:	Westbridge Agricultural Products
Company Agent:	Frederick T. Smith
Title:	Agent*
Signature:	
Date:	3/28/13

*SciReg, Inc. is the authorized agent for Westbridge Agricultural Products

GOOD LABORATORY PRACTICES COMPLIANCE STATEMENT

The material presented in this section is not a study but a presentation of factual information and is, therefore, not subject to GLP requirements. This report is a compilation of technical information and it did not have a Study Director.

Sponsor/Submitter: [signature]

Date: 3/28/13

Mammalian Toxicity Profile of Capric Acid (Decanoic Acid)

OPPTS Test Guidelines: 870.1100 – 870.5375

Capric Acid (Decanoic Acid)

Per the Agency's Capric Acid Final Work Plan, EPA does not have any formal guideline toxicology studies for capric acid (C10). Instead, open literature studies and information were determined to be acceptable. These and other data are summarized below.

1. **Acute oral toxicity (870.1100)**
   Capric Acid LD50: >10 g/kg (Capric Acid Final Registration Review Decision; 1)

2. **Acute dermal toxicity (870.1200)**
   Capric Acid LD50: >5 g/kg (Capric Acid Final Registration Review Decision; 1)

3. **Acute inhalation toxicity (870.1300)**
   a. Groups of six rats were exposed to concentrated mixed octanoic acid isomers for up to 4 hours. All animals survived. (IUCLID Dataset; 2)

   b. MRID No. 40943008

4. **Primary eye irritation (870.2400)**
   Capric acid is a severe eye irritant when applied as a 5% dilution. (Capric Acid Final Registration Review Decision; 1)

5. **Primary skin irritation (870.2500)**
   Capric acid is a moderate to severe skin irritant when applied undiluted to intact or abraded rabbit skin for 24 hours. (Capric Acid Final Registration Review Decision; 1)

6. **Dermal sensitization (870.2600)**
   a. Capric acid was evaluated in a Buehler test. Twenty treated (capric acid in ethanol) and 10 control animals were used. Test animals were treated once per week for six hours under a closed patch, followed by two weeks of rest. The challenge application was administered to all animals at a virgin test site using capric acid and acetone. No sensitization was observed. (IUCLID Dataset; 2)

7. **Hypersensitivity incidents (no guideline number)**
   During the course of product development and in-house evaluation of BioLink Herbicide, various personnel have been working intimately with the active ingredient and finished formulation. There have been no issues with hypersensitivity to the active ingredients or the finished formulation.

8. **90-day oral toxicity (870.3100)**
   a. Rats fed capric (decanoic) acid at 10% in the diet for 150 days showed no adverse effects from treatment. (Capric Acid Final Registration Review Decision; 1)

b. Rats administered approximately 4 g capric acid/kg/day for 6 weeks showed reduced body weight gain and increased plasma triglyceride levels. (Capric Acid Final Registration Review Decision; 1)

c. In a longer term study in which rats were fed 2.5 g/kg/day capric acid for 47 weeks, no abnormalities of the cellular structure of the liver or intestine were noted. (Capric Acid Final Registration Review Decision; 1)

d. Dogs administered 4.4 g/kg/day capric acid for 102 days showed no adverse effects from treatment. (Capric Acid Final Registration Review Decision; 1)

9. 90-day dermal toxicity (870.3250)

In a subchronic study, no adverse effects were produced from topical application of myristic acid (C14) to rabbit skin. One-half ml of a 30% preparation of myristic acid in ether and propylene glycol (solvents at a 1:1 ratio) was massaged into the depilated skin of the flanks of 5 rabbits daily for 30 days. The opposite flank of the rabbits was depilated and treated with solvent only. No significant macroscopic changes were observed. Microscopic lesions included thinning of collagen fibres in the superficial layer of the dermis after 10 days and a loose dermal infiltrate of lymphomononuclear cells and histocytes after 20 and 30 days. (HERA, 2002; 3)

10. 90-day inhalation toxicity (870.3465)

There are no publically-available subchronic inhalation data on capric acid. However, given the low order of toxicity of fatty acids as a group and their long history of safe use, inhalation exposure should not be a concern. Further, the fact that the registrant, Westbridge Agricultural Products, does not intend to sell or distribute this product and, therefore, very limited internal personnel only are potentially exposed to this product, inhalation exposure is not problematic.

11. Developmental toxicity (870.3700)

a. Medium chain triglycerides (MCTs) are a family of triglycerides, containing predominantly, caprylic [C(8)] and capric [C(10)] fatty acids with lesser amounts of caproic [C(6)] and lauric [C(12)] fatty acids. There was no evidence that intravenous (iv) or dietary administration of MCTs adversely affected the reproductive performance of rats or resulted in maternal toxicity, fetal toxicity, or teratogenic effects at doses up to 4.28 g/kg body weight/day (iv) or 12,500 mg/kg body weight/day (dietary). There was no evidence that dietary administration of MCTs adversely affected the reproductive performance of pigs or resulted in maternal toxicity, fetal toxicity or teratogenic effects at doses up to 4000 mg/kg body weight/day in the diet. In rabbits, following iv administration, the maternal and fetal no-observed-adverse-effect levels (NOAELs) were between 1.0 and 4.28 g/kg body weight/ day. **PEER REVIEWED** (Hazardous Substances Data Bank; 4)

12. Bacterial reverse mutation assay (870.5100)

a. Capric acid (0 to 666 ug/plate) gave negative results in *Salmonella typhimurium* strain TA 97, TA 98, TA 100, TA 1535, and TA 1537 with or without metabolic activation. **PEER REVIEWED** (IUCLID Dataset; 2)

b. In an *Escherichia coli* reverse mutation assay, capric acid was applied to agar plates innoculated with various concentrations of *E. coli* strain Sd-4-73 (streptomycin-dependent). Capric acid was either applied directly to the agar or on filter paper disc. No mutagenic activity was reported. **PEER REVIEWED** (IUCLID Dataset; 2)

c. MRID 40943005

13. *In vitro* mammalian cell assay (870.5300/870.5895)

a. Chromosome aberration (MRID 40943006)

b. Unscheduled DNA synthesis (MRID 40943007)

References

1. Environmental Protection Agency Capric Acid Final Registration Review Decision, 2009.

2. IUCLID Dataset: Decanoic Acid. European Commission, European Chemicals Bureau, 2000.

3. Human & Environmental Risk Assessment on Ingredients of European Household Cleaning Products: Fatty Acid Salts. Human Health Risk Assessment, 2002.

4. Hazardous Substances Data Bank: Decanoic Acid.

REFERENCE 1

Docket Number: EPA-HQ-OPP-2007-1040
www.regulations.gov

United States Environmental Protection Agency | Prevention, Pesticides and Toxic Substances (7510P) | March 2009

EPA

Capric (Decanoic) Acid
Final Registration Review Decision
Registration Review Case 5038

Docket Number EPA-HQ-OPP-2007-1040

Capric (Decanoic) Acid
Final Registration Review Decision
Registration Review Case 5038

Approved by: Joan Harrigan-Farrelly

Joan Harrigan-Farrelly, Director
Antimicrobials Division

Date: 2/19/09

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Final Registration Review Decision for
Capric (Decanoic) Acid, Case 5038

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I. INTRODUCTION

This document is EPA's Final Registration Review Decision for Capric (Decanoic) Acid and is being issued pursuant to 40 CFR Sections 155.57 and 155.58. A registration review decision is the Agency's determination whether a pesticide meets, or does not meet, the standard for registration in the Federal Insecticide, Fungicide and Rodenticide Act (FIFRA). For additional information on Capric (Decanoic) Acid, additional documents can be found in EPA's public docket (EPA-HQ-OPP-2007-1040) at www.regulations.gov.

FIFRA, as amended by the Food Quality Protection Act (FQPA) of 1996, mandated the continuous review of existing pesticides. All pesticides distributed or sold in the United States must generally be registered by EPA, based on scientific data showing that they will not cause unreasonable risks to human health (including occupational and non-occupational exposures) or the environment when used as directed on product labeling. The new registration review program is intended to make sure that, as the ability to assess risk evolves and as policies and practices change, all registered pesticides continue to meet the statutory standard of no unreasonable adverse effects to human health or the environment. Changes in science, public policy, and pesticide use practices will occur over time. Through the new registration review program, the Agency periodically reevaluates pesticides to make sure that as change occurs, products in the marketplace can be used safely. Information on this program is provided at: http://www.epa.gov/oppsrrd1/registration_review/.

In 2006, the Agency implemented the Registration Review program pursuant to FIFRA Section 3(g) and will review each registered pesticide every 15 years to determine whether it continues to meet the FIFRA standard for registration.

Pursuant to 40 CFR Sec. 155.50, the Agency formally initiated registration review for Capric (Decanoic) Acid with the following timeline:

- December 2007 – publication of a Preliminary Work Plan (PWP) in the initial docket for Capric (Decanoic) Acid (EPA-HQ-OPP-2007-1040). During the 90 day comment period that closed on March 11, 2008, the Agency received no comments from the public.
- August 2008 – Issuance of a Final Work Plan and Proposed Registration Review Final Decision stating that the most recent exposure and risk assessments still supported the registration of pesticide products containing Capric (Decanoic) Acid and meet the requirements of registration review under 40 CFR Sec. 155.50. This document was issued for a 60-day public comment period; no comments were received.
- February 2009 – Issuance of a Final Registration Review Decision.

No comments were received on the Preliminary Work Plan (PWP), issued in December 2007, or the combined Final Work Plan and Proposed Registration Review Final Decision, issued in August 2008. The Agency is making its final decision on Capric (Decanoic) Acid based on no comments having been received and the low toxicity of Capric (Decanoic) Acid. In addition, the data and information evaluated to support Capric (Decanoic) Acid, case 5038, as published in the PWP dated December 12, 2007, continue to support this pesticide registration as summarized herein. The status of these and other registration review cases is available on *http//www.epa.gov/oppsrrd1/registration review/ review.*

Capric (Decanoic) Acid, also referred to as decanoic acid, is an antimicrobial pesticide that is used as a food contact surface sanitizer in commercial food handling establishments. In addition, Capric (Decanoic) Acid is characterized by low toxicity, is biodegradable, and is found extensively in nature.

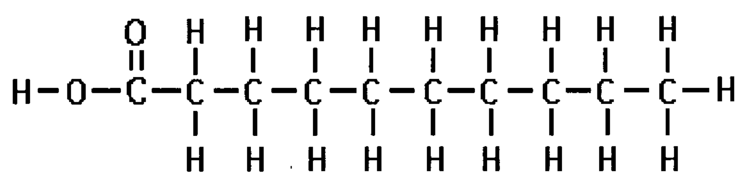
Currently, there are four registered products containing Capric (Decanoic) Acid as an active ingredient. This Registration Review of Capric (Decanoic) Acid addresses the Capric (Decanoic) Acid component of the registered products. The other active ingredients will be addressed during their subsequent Registration Review. Due to the products' registered uses on dairy and food-processing equipment such as tanks, vats, pails, pipelines and closed systems, there is the potential for residues in food; thus, Capric (Decanoic) Acid is considered to be a food-use chemical under the Federal Food, Drug, and Cosmetic Act (FFDCA). However, an exemption from the requirement of a tolerance for residues of Capric (Decanoic) Acid in foods has been established (40 CFR 180.1225).

II. SCIENTIFIC ASSESSMENT

A. Chemical Identification

Table 1 provides information on the chemical identity of Capric (Decanoic) Acid.

Table 1. Chemical Identity

Common Name	Capric (Decanoic) Acid
Chemical Name	n-Decanoic Acid
Molecular Weight	172.27
PC Code	128955
CAS Registry Number	334-48-5
Empirical Formula	$C_{10}H_{20}O_2$
Registration Review Case No.	5038
Chemical Structure: $CH_3(CH2)_8COOH$	 Capric Acid

B. Product Chemistry

Table 2 provides information on the physical and chemical properties of Capric (Decanoic) Acid. All product chemistry data requirements have been fulfilled for the active ingredient Capric (Decanoic) Acid; no additional data are needed at this time.

Table 2. Product Chemistry Data Summary for Capric (Decanoic) Acid

Guideline No.	Physical and Chemical Properties	Status	Value
830.1550	Product identity and composition	Acceptable	Refer to Table 1
830.1600	Description of materials used to produce the product	Acceptable	CBI
830.1620	Description of production process	Acceptable	CBI
830.1650	Description of formulation process	Acceptable	CBI
830.1670	Discussion of formation of impurities	Acceptable	CBI
830.1700	Preliminary analysis	Acceptable	CBI
830.1750	Certified limits	Acceptable	CBI
830.1800	Enforcement analytical method	Acceptable	Gas-Liquid Chromatography
830.1900	Submittal of samples	N/A	
830.6302	Color	Acceptable	White Crystals
830.6303	Physical State	Acceptable	Clear, Colorless Liquid White Crystalline Solid
830.6304	Odor	Acceptable	Unpleasant Musty, Rancid
830.6313	Stability to sunlight, normal and elevated temperature, metals/metal ions	Acceptable	Stable. Stable at room temperature in closed containers under normal storage and handling conditions. Presents no notable stability hazard other than low fire hazard (flash point = 270°F).
830.6314	Oxidation/Reduction: Chemical Incompatibility	Acceptable	Avoid strong oxidizing agents.
830.6315	Flammability	Acceptable	Flash Point: 112°C
830.6316	Explodability	Acceptable	Non-explodable
830.6317	Storage Stability	Acceptable	Stable at room temperature and no change in composition over the eighteen months storage.
830.6319	Miscibility	N/A	Not meant for dilution with petroleum solvents.
830.6320	Corrosion Characteristic	Acceptable	Non-corrosive
830.6321	Dielectric breakdown voltage	N/A	Not intended for use in or around electrical equipment.
830.7000	pH	Acceptable	Not soluble in water
830.7050	UV/Visible absorption	N/A	
830.7100	Viscosity	Acceptable	2.88 mPa.s at 70°C 4.30 mPa.s (cP) at 50°C (TOXNET)
830.7200	Melting Point	Acceptable	31.2 - 31.6°C
830.7220	Boiling point	Acceptable	270°C (760 mm Hg) 148-150°C (11 mm Hg)
830.7300	Density	Acceptable	1.02 gm/ml at 25°C (0.893 g/cm3) 0.8858 at 40°C

Guideline No.	Physical and Chemical Properties	Status	Value
830.7300	Specific Gravity	Acceptable	0.9
830.7370	Dissociation Constants in water	Acceptable	Not determined due to lack of solubility in water. 4.90 (TOXNET)
830.7550	Octanol/water partition coefficient	Acceptable	This active ingredient is a non-polar organic substance. Log Kow: 4.09 (EPI Suite)
830.7840	Solubility in water (g/100ml)	Acceptable	0.015 gm/l00gm at 20°C 0.15 g/liter (20°C) Practically insoluble in water
830-xxxx	Solubility in organic solvents		Acetone (20°C) = 407 gm/l00gm Isopropanol (20°C) = 360 gm/l00gm Methanol (20°C) 510 gm/l00gm n-hexane (20°C) = 290 gm/l00gm Soluble in alcohol and ether.
830.7950	Vapor pressure	Acceptable	Not Applicable. Melting point greater than 30°C. 0.00878 mm Hg (EPI Suite) Less than 1 mm Hg at 72°F 0.13 hPa @ 79°C
	Hazardous Decomposition Products		Does not decompose up to 400°F
	Hazardous Polymerization		Does not occur
Other Physical/Chemical Properties			
	Classification of a.i.		Aliphatic hydrocarbon Carboxylic acid
	Henry's Law Constant at 25°C		1.342E-006 atm-m3/mole (EPI Suite)
	Koc		Estimated Koc: 87.2 (EPI Suite) Log Koc: 1.9403 (EPI Suite)
	Ready Biodegradability Prediction		Yes (EPI Suite) Microbiological degradation.
	Hydrolysis		No hydrolysis
	Log BCF		Log BCF = 0.500 (EPI suite) BCF=3.162 (EPI suite)
	Refractive Index		1.4569 (20°C)

C. Human Health Risk Assessment Status

1. Toxicology

The Agency does not have formal guideline toxicology studies for Capric (Decanoic) Acid. The information presented herein has been gathered from the open scientific literature.

a. Acute Toxicity

From the BIBRA Information Services Ltd. (http://www.bibra-information.co.uk/) Toxicity Profile for Capric (Decanoic) Acid, the acute oral toxicity is low (LD_{50} >10 g/kg) as is the acute dermal toxicity (LD_{50} >5 g/kg). Capric (Decanoic) Acid is a moderate to severe skin irritant when applied undiluted to intact or abraded rabbit skin for 24 hours. Capric (Decanoic) Acid is also a severe eye irritant when applied as a 5% solution.

b. Subchronic and Chronic Toxicity

As reported in Patty's Industrial Hygiene and Toxicology, 4th ed., rats fed Capric (Decanoic) Acid at 10% in the diet for 150 days showed no adverse effects from treatment. In a study by Renaud et al. (Journal of Nutrition, Vol. 90, 1966, p. 453) rats administered approximately 4 g Capric (Decanoic) Acid/kg/day for 6 weeks showed reduced body weight gain and increased plasma triglyceride levels. In a longer term study in which rats were fed 2.5 g/kg/day Capric (Decanoic) Acid for 47 weeks, no abnormalities of the cellular structure of the liver or intestine were noted. Dogs administered 4.4 g/kg/day Capric (Decanoic) Acid for 102 days showed no adverse effects from treatment.

In another study by Hendrich et. al., (JAOCS, Vol. 70, no. 8, August 1993, pages 797-802), CBA/2 and C57B1/6 mice were fed *Cuphea* oil containing 76% Capric (Decanoic) Acid. The control diet contained beef tallow, and the *Cuphea* oil diet substituted for half of the beef tallow in the experimental diet. Although the study design is not very clear, it appears that parental animals were fed for various times due to the short supply of *Cuphea* oil. C57B1/6 mice were fed for either 10 months, 8 months, or 5 months (F1, F2, and F3 generations), while the CBA/2 mice were fed for 11-12 months, 9-11 months, and 6-8 months (F1, F2, and F3 generations). Body weights, food intake, liver weights, and total serum cholesterol were analyzed as well as the number of pups born and surviving to weaning. Histopathology was performed on liver, left kidney, spleen, heart, lung, and one testis. The histopathology appears to have been done only on parental mice. Feeding of *Cuphea* oil containing Capric (Decanoic) Acid to successive generations of two strains of mice did not appear to affect reproductive parameters. There was an unexplained drop in the number of pups surviving to weaning in the F1 and F2 generations for both strains of mice. Body weight in C57B1/6 and CBA/2 mice was reduced approximately 10% after 13 weeks of treatment but this effect was not observed in successive generations. Food intake was not consistently affected by treatment. Serum cholesterol was significantly increased in C57B1/6 mice after 3 months of treatment, and the increase was also observed after 5 and 12 months. Fatty vacuolization was observed in the liver of most mice after treatment. CBA/2 mice tended to accumulate fat as large vacuoles in periportal hepatocytes with smaller vacuoles in centrilobular hepatocytes. C57B1/6 mice had a more diffuse fatty change with large vacuoles in centrilobular areas.

c. Carcinogenicity

There are no available data on carcinogenicity of Capric (Decanoic) Acid. However, available mutagenicity data (Negishi and Hayatsu, Mut. Res. 135: 87-96, 1984) show Capric (Decanoic) Acid inhibits N-nitrosodimethylamine induced mutagenesis by virtue of its antimicrobial activity.

d. Physiological Effects

Capric (Decanoic) Acid was observed to enhance the permeability of the blood-brain barrier in Wistar rats to several hydrophilic compounds when administered into the carotid artery (Ohnishi et al., J. Pharm. Pharmacol. 51: 1015-1018, 1998).

e. Endocrine Effects

The Agency is required under section 408(p) of the Federal Food, Drug and Cosmetic Act (FFDCA), as amended by FQPA, to develop a screening program to determine whether certain substances (including all pesticide active and other ingredients) "may have an effect in humans that is similar to an effect produced by a naturally-occurring estrogen, or other such endocrine effect as the Administrator may designate." Following the recommendations of its Endocrine Disruptor Screening and Testing Advisory Committee (EDSTAC), EPA determined that there was a scientific basis for including, as part of the program, androgen and thyroid hormone systems, in addition to the estrogen hormone system. EPA also adopted EDSTAC's recommendation that it include evaluations of potential effects in wildlife. The Agency does not have any information with respect to potential endocrine effects of Capric (Decanoic) Acid in mammalian systems. There is no information from the available scientific literature to suggest that this fatty acid would have endocrine effects.

The Agency has no knowledge of Capric (Decanoic) Acid being an endocrine disruptor. When the appropriate screening and/or testing protocols being considered under the Agency's Endocrine Disrupter Screening Program (EDSP) have been developed and vetted, Capric (Decanoic) Acid may be subjected to additional screening and/or testing to better characterize effects related to endocrine disruption.

Although the toxicity data base for Capric (Decanoic) Acid is limited, the toxicity profile indicates no significant systemic toxicity even at high dose levels. Therefore, a quantitative assessment is not being conducted and no human health toxicity endpoints for the active ingredient Capric (Decanoic) Acid have been selected. The Agency does not anticipate the need for additional toxicity or exposure data for Capric (Decanoic) Acid.

2. Dietary, Drinking Water, Residential and Occupational Exposure

a. Dietary Exposure

An exemption from the requirement of a tolerance for residues has been established in 40 CFR 180.1225 and 40 CFR 180.940 (b) and (c) because no adverse systemic effects attributable to oral exposure have been identified. Based on the registered uses as a sanitizer on dairy equipment and in food processing equipment such as tanks, vats, pails, pipelines and closed systems, minimal dietary exposure is expected to occur from Capric (Decanoic) Acid use. Therefore, dietary exposure and risk will not be assessed for Capric (Decanoic) Acid when used as a food contact surface sanitizer.

b. Drinking Water Exposure

As all registered use sites are indoors, no dietary exposure from drinking water is expected to occur from residential wells or municipal sources. However, there is a possibility that the use of Capric (Decanoic) Acid as a surface sanitizer in water bottling plants may result in the occurrence of low concentrations in bottled drinking water. Because of the low toxicity associated with Capric (Decanoic) Acid, and the existing tolerance exemptions, the risk of dietary exposure from drinking water is not of concern.

c. Residential and Occupational Exposure

Based on the registered uses of Capric (Decanoic) Acid as a food contact surface sanitizer in food handling establishments, no potential residential exposure is anticipated. Because of the low toxicity of Capric (Decanoic) Acid, adverse effects from Capric (Decanoic) Acid are not expected. Occupational exposure to workers who mix, load, and apply Capric (Decanoic) Acid is expected; however, a risk assessment is not needed based on the low toxicity.

D. Environmental Fate and Ecological Effects Exposure and Risk Assessment Status

1. Environmental Fate

An environmental fate assessment has not been conducted for Capric (Decanoic) Acid. Capric (Decanoic) Acid is classified as a saturated fatty acid, a group of substances which is completely biodegradable and found extensively in nature. Specifically, Capric (Decanoic) Acid occurs in a number of plants, and animal sources such as animal oils, fats, butter, coconut oil, etc. It is a food-grade substance, non-volatile and relatively inert to aqueous hydrolysis. It is a minimal risk and low concern inert, a normal constituent in animal diet and is readily metabolized by all forms of life. Microorganisms rapidly degrade fatty acids in soil. Thus, the Agency does not anticipate the need for a down-the-drain assessment and does not anticipate risks of concern to wastewater treatment plants (WWTPs).

2. Ecological Effects

The Agency has conducted a review of the scientific databases and other relevant information supporting the reregistration of Capric (Decanoic) acid, and has waived all generic data requirements for this chemical. Capric (Decanoic) acid is listed as Generally Recognized as Safe (GRAS) food additive by the Food and Drug Administration (21 CFR 172.863; as food additives permitted for direct addition to food for human consumption). Fatty acids normally are metabolized, forming simple compounds that serve as energy sources and structural components used in all living cells. Capric (Decanoic) Acid ($C_{10}H_{20}O_2$) is structurally similar to Lauric acid ($C_{12}H_{24}O_2$), Myristic acid ($C_{14}H_{28}O_2$), Oleic acid ($C_{18}H_{34}O_2$) and Ricinoleic acid ($C_{18}H_{34}O_3$) except for the different carbon chain length.

3. Endangered Species

As mentioned previously, Capric (Decanoic) Acid has low toxicity. There are four products registered for pesticidal use; these products are registered for indoor use and have a low percentage of this active ingredient in the end use product (≤3% ai). In addition, Capric (Decanoic) Acid is classified as a saturated fatty acid, a group of substances which is completely biodegradable and found extensively in nature. It is naturally occurring in vegetable oils and in animal fats and is a significant part of the normal diets of mammals, birds and invertebrates; it is readily metabolized by all forms of life.

Capric (Decanoic) Acid is not expected to contaminate ground water or soil and does not accumulate in the food chain. Because of the rapid degradation of Capric (Decanoic) Acid into components that do not pose a risk to aquatic organisms, the Agency is not conducting a down-the-drain assessment.

Based on rapid decomposition, indoor use patterns, no-to-extremely low environmental exposure potential, and low toxicity, the Agency has determined that the registered uses of Capric (Decanoic) Acid will have "no effect" (NE) on endangered or threatened terrestrial or aquatic species, or their designated critical habitats, as listed by the U.S. Fish and Wildlife Service (USFWS) and the National Oceanic and Atmospheric Administration (NOAA).

E. Incidents

Federal law requires registrants of pesticides to inform EPA about any harmful effects of their products. There are 8 incidents for products containing Capric (Decanoic) Acid that were found during a search of the OPP Incident Data System (IDS), containing data collected from 1992-present. These incidents reported that exposure caused minor to moderate irritation reactions. Dermal and eye exposure caused rash, redness, pain, diarrhea, chemical burns, corneal abrasion, heavy breathing, headache, dizziness, vertigo, vomiting, and swelling esophagus. Oral ingestion caused abdominal pain and throat discomfort.

It should be noted that each product currently registered containing Capric (Decanoic) Acid contains at least one other active ingredient in higher concentration. At least one other active ingredient in every implicated Capric (Decanoic) Acid-containing end-use product is expected to be more severely irritating than Capric (Decanoic) Acid, especially at the concentrations formulated. Based on the low number of incidents reported for products containing Capric (Decanoic) Acid, and the low toxicity of Capric (Decanoic) Acid, the Agency believes that these incident reports may not indicate a specific Capric (Decanoic) Acid-related cause.

F. Public Comments

Pursuant to 40 CFR Sec. 155.50, the Agency formally initiated registration review for Capric (Decanoic) Acid on December 12, 2007 with the opening of a docket and the issuance of a PWP for public comment. The Agency received no comments concerning the Preliminary

Work Plan for Capric (Decanoic) Acid during its 90-day public comment period. The Agency also received no comments concerning the Combined Final Work Plan and Proposed Registration Review Final Decision document issued for a 60-day public comment period on August 29, 2008.

G. Environmental Justice

EPA seeks to achieve environmental justice - the fair treatment and meaningful involvement of all people, regardless of race, color, national origin, or income - in the development, implementation, and enforcement of environmental laws, regulations, and policies. At this time EPA does not believe that use of pesticide products containing Capric (Decanoic) Acid will cause harm or a disproportionate impact on at-risk communities. In the Preliminary Work Plan dated December 12, 2007, the Agency sought comment on environmental justice issues regarding Capric (Decanoic) Acid. As mentioned previously, no comments were received.

For additional information regarding environmental justice issues, please visit EPA's website at: http://www.epa.gov/compliance/environmentaljustice/index.html.

H. Water Quality

Capric (Decanoic) Acid is not identified as a cause of impairment for any water-bodies listed as impaired under section 303(d) of the Clean Water Act, based on information provided at: http://oaspub.epa.gov/tmdl/waters_list.impairments?p_impid=3. The Agency sought submission of water quality information for Capric (Decanoic) Acid when the Preliminary Work Plan was issued for comment. The Agency did not receive any comments on water quality issues.

I. Trade Irritants

Through the registration review process, the Agency solicited information on trade irritants and, to the extent feasible, took steps toward facilitating irritant resolution. Growers and other stakeholders were asked to comment on any trade irritant issues resulting from lack of Maximum Residue Levels (MRLs) or disparities in key export markets, providing as much specificity as possible regarding the nature of the concern. In the case of Capric (Decanoic) Acid, there are indirect food uses as Capric (Decanoic) Acid is registered for use as a contact surface sanitizer in commercial food handling establishments. In addition, an exemption from the requirement of a tolerance for residues has been established in 40 CFR 180.1225 and 40 CFR 180.940 (b) and (c). Additionally, there are no MRLs established for Capric (Decanoic) Acid. The Agency did not receive and comments regarding the existence of any trade irritant issues associated with Capric (Decanoic) Acid.

III. FINAL REGISTRATION REVIEW DECISION

The Agency has determined that no additional data are required at this time to support the registration of Capric (Decanoic) Acid. The Agency has considered Capric (Decanoic) Acid in light of the standard for registration and safety factors in FIFRA and FFDCA as amended by FQPA. EPA has found that there are not likely to be any unreasonable adverse effects to the U.S. population in general, and to infants and children in particular, or to non-target organisms or the environment, from the use of registered pesticide products containing Capric (Decanoic) Acid when currently required label instructions are followed. The Agency has found that it is not necessary to conduct a new risk assessment for this case and is therefore issuing a proposed final decision pursuant to 40 CFR 155.53 (c)(2) and 40 CFR 155.58.

As per 40 CFR Sections 155.57 and 155.58, the Agency determined that the standards for Registration Review have been met, and the registrations of the aforesaid Capric (Decanoic) Acid products may be maintained.

IV. NEXT STEPS AND TIMELINE:

Pursuant to 40 CFR Section 155.58, this Final Registration Review Decision document is being entered into the Capric (Decanoic) Acid docket (EPA-HQ-OPP-2007-1040). The Final Work Plan is also included in this document. A Federal Register Notice will announce the availability of the Final Registration Review Decision.

V. GLOSSARY of TERMS & ABBREVIATIONS

ai	Active Ingredient
AR	Anticipated Residue
ASTM	American Society for Testing and Materials
AWPA	American Wood Preserver's Association
CFR	Code of Federal Regulations
cPAD	Chronic Population Adjusted Dose
CSF	Confidential Statement of Formula
CSFII	USDA Continuing Surveys for Food Intake by Individuals
DCI	Data Call-In
DEEM	Dietary Exposure Evaluation Model
DFR	Dislodgeable Foliar Residue
DNT	Developmental Neurotoxicity
DWLOC	Drinking Water Level of Comparison
EC	Emulsifiable Concentrate Formulation
EDWC	Estimated Drinking Water Concentration
EEC	Estimated Environmental Concentration
EPA	Environmental Protection Agency
EUP	End-Use Product
FDA	Food and Drug Administration
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FFDCA	Federal Food, Drug, and Cosmetic Act
FQPA	Food Quality Protection Act
FOB	Functional Observation Battery
GENEEC	Tier I Surface Water Computer Model
IR	Index Reservoir
LC_{50}	Median Lethal Concentration. A statistically derived concentration of a substance that can be expected to cause death in 50% of test animals. It is usually expressed as the weight of substance per weight or volume of water, air or feed, e.g., mg/l, mg/kg or ppm.
LD_{50}	Median Lethal Dose. A statistically derived single dose that can be expected to cause death in 50% of the test animals when administered by the route indicated (oral, dermal, inhalation). It is expressed as a weight of substance per unit weight of animal, e.g., mg/kg.
LOC	Level of Concern
LOAEL	Lowest Observed Adverse Effect Level
μg/g	Micrograms Per Gram
μg/L	Micrograms Per Liter
mg/kg/day	Milligram Per Kilogram Per Day
mg/L	Milligrams Per Liter
MOE	Margin of Exposure
MRID	Master Record Identification (number). EPA's system of recording and tracking submitted studies.
MUP	Manufacturing-Use Product
NA	Not Applicable
NAWQA	USGS National Ambient Water Quality Assessment
NPDES	National Pollutant Discharge Elimination System
NR	Not Required
NOAEL	No Observed Adverse Effect Level
OPP	EPA Office of Pesticide Programs
OPPTS	EPA Office of Prevention, Pesticides and Toxic Substances
PAD	Population Adjusted Dose
PAIRA	Pure Active Ingredient Radiolabelled
PCA	Percent Crop Area
PDP	USDA Pesticide Data Program

PHED	Pesticide Handler's Exposure Data
PHI	Preharvest Interval
ppb	Parts Per Billion
PPE	Personal Protective Equipment
ppm	Parts Per Million
PRZM/EXAMS	Tier II Surface Water Computer Model
Q_1*	The Carcinogenic Potential of a Compound, Quantified by the EPA's Cancer Risk Model
RAC	Raw Agriculture Commodity
RED	Reregistration Eligibility Decision
REI	Restricted Entry Interval
RfD	Reference Dose
RQ	Risk Quotient
SCI-GROW	Tier I Ground Water Computer Model
SAP	Science Advisory Panel
SF	Safety Factor
SLN	Special Local Need (Registrations Under Section 24©) of FIFRA)
TGAI	Technical Grade Active Ingredient
TEP	Typical End-Use Product
USDA	United States Department of Agriculture
UF	Uncertainty Factor
WPS	Worker Protection Standard

REFERENCE 2

I U C L I D

D a t a s e t

Existing Chemical	Substance ID: 334-48-5
CAS No.	334-48-5
EINECS Name	decanoic acid
EINECS No.	206-376-4
Molecular Weight	172.27
Structural Formula	CH3-(CH2)8-COOH
Molecular Formula	C10H20O2

Dataset created by: EUROPEAN COMMISSION - European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non-confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

Creation date: 18-FEB-2000

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Chapters: all

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Flags: non-confidential

1.0.1 OECD and Company Information

Name: Henkel KGaA
Street: Henkelstr. 67
Town: 40589 Duesseldorf
Country: Germany

Name: Krahn Chemie
Street: Grimm 10
Town: 20457 Hamburg
Country: Germany
Phone: 040 320920
Telefax: 040 32092219

Name: Procter & Gamble UK (Hayes)
Street: P.O. Box 9, Hayes Gate House, 27 Uxbridge Road
Town: UB4 0JD Middlesex
Country: United Kingdom

Name: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Street: Ueberseering 40
Town: 22297 Hamburg
Country: Germany
Phone: 040-6375-0
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Telex: 21151320

Name: Unichema Chemie GmbH
Street: Steintor 9
Town: D-46446 Emmerich
Country: Germany
Phone: +49-2822-720
Telefax: +49-2822-72276

1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

-

1.1 General Substance Information

Substance type: organic
Physical status: liquid

Substance type: organic
Physical status: solid

1.1.1 Spectra

-

1.2 Synonyms

1-nonane carboxylic acid
Source: Unichema Chemie GmbH Emmerich

1-Nonanecarboxylic acid
Source: Henkel KGaA Duesseldorf

C-1095
Source: Henkel KGaA Duesseldorf

C10 Fatty acid
Remark: See lead Hedset
Source: Procter & Gamble UK (Hayes) Middlesex

Capric Acid
Source: Henkel KGaA Duesseldorf

Capric acid (INCI name)
Source: Unichema Chemie GmbH Emmerich

Capric acid (INCI)
Source: Henkel KGaA Duesseldorf

Capric acid, Decylic acid, Decoid acid, n-decanoic acid, 1-nonane carboxylic acid, Caprinic acid, Hexacid 1095
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

Caprinic acid
Source: Henkel KGaA Duesseldorf
Unichema Chemie GmbH Emmerich

Caprinsäure
Source: Henkel KGaA Duesseldorf

Caprynic acid
Source: Henkel KGaA Duesseldorf

Decanoic acid
Source: Henkel KGaA Duesseldorf

DECANSAEURE
Source: Henkel KGaA Duesseldorf

DECANSAEURE (ALTSTOFF)
Source: Henkel KGaA Duesseldorf

Decansäure
Source: Henkel KGaA Duesseldorf

DECANsäure (ALTSTOFF)
Source: Henkel KGaA Duesseldorf

Decatoic acid
Source: Unichema Chemie GmbH Emmerich

Decoic acid
Source: Henkel KGaA Duesseldorf
Unichema Chemie GmbH Emmerich

Decylic acid
Source: Henkel KGaA Duesseldorf
Unichema Chemie GmbH Emmerich

Docansäure
Source: Henkel KGaA Duesseldorf

Emery 659
Source: Henkel KGaA Duesseldorf

Hexacid 1095
Source: Unichema Chemie GmbH Emmerich

Lunac 10-95
Source: Henkel KGaA Duesseldorf

n-Capric Acid
Source: Henkel KGaA Duesseldorf

n-Decanoic acid
Source: Henkel KGaA Duesseldorf

n-decanoic acid
Source: Unichema Chemie GmbH Emmerich

n-Decoic acid
Source: Henkel KGaA Duesseldorf

n-Decylic acid
Source: Henkel KGaA Duesseldorf

NAA 102
Source: Henkel KGaA Duesseldorf

Prifac 2906
Source: Henkel KGaA Duesseldorf

Prifac 296
Source: Henkel KGaA Duesseldorf

Prifrac 2906
Source: Henkel KGaA Duesseldorf

Source: Henkel KGaA Duesseldorf

1.3 Impurities

-

1.4 Additives

-

1.5 Quantity

Quantity 10 000 - 50 000 tonnes

1.6.1 Labelling

-

1.6.2 Classification

-

1.7 Use Pattern

Type: type
Category: Use in closed system

Type: type
Category: Use resulting in inclusion into or onto matrix

Type: industrial
Category: Basic industry: basic chemicals

Type: industrial
Category: Chemical industry: used in synthesis

Type: industrial
Category: Paints, lacquers and varnishes industry

Type: industrial
Category: Personal and domestic use

Type: industrial
Category: other

Type: use
Category: Cosmetics

Type: use
Category: Intermediates

Type: use
Category: Solvents

Type: use
Category: other: base for wetting agent

Type: use
Category: other: esters for perfumes and flavors

Type: use
Category: other: esters for perfumes and flavours

1.7.1 Technology Production/Use

-

1.8 Occupational Exposure Limit Values

Type of limit:
Limit value:
Remark: Not established;
goggles or face shield recommended for eye protection
and rubber or plastic gloves recommended
for hand protection.
Source: Procter & Gamble UK (Hayes) Middlesex

Type of limit:
Limit value:
Remark: not established
Source: Unichema Chemie GmbH Emmerich

(1)

1.9 Source of Exposure

-

1.10.1 Recommendations/Precautionary Measures

-

1.10.2 Emergency Measures

-

1.11 Packaging

-

1.12 Possib. of Rendering Subst. Harmless

-

1.13 Statements Concerning Waste

-

1.14.1 Water Pollution

Classified by: KBwS (DE)
Labelled by:
Class of danger: 1 (weakly water polluting)
Remark: German Commission for the Assessment of Water Polluting Substances (Datasheet No. 657)
Source: Transfer program
Henkel KGaA Duesseldorf

Classified by: KBwS (DE)
Labelled by: KBwS (DE)
Class of danger: 1 (weakly water polluting)
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

1.14.2 Major Accident Hazards

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Source: Henkel KGaA Duesseldorf

Legislation: Stoerfallverordnung (DE)
Substance listed: no
Remark: Katalog wassergefaehrende Stoffe, Datenlatt Nr. 657, 1988.
Source: RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

1.14.3 Air Pollution

-

1.15 Additional Remarks

Remark: MAJOR ACCIDENT HAZARDS
Legislation : Störfallverordnung (DE)
Substance listed: No
WATER POLLUTION
Classified by: KBwS
Labelled by : KBwS
Class of danger: 1
Source: Unichema Chemie GmbH Emmerich

(2)

1.16 Last Literature Search

-

1.17 Reviews

-

1.18 Listings e.g. Chemical Inventories

-

2.1 Melting Point

Value: 30.5 - 32 degree C
Decomposition: no
Sublimation: no
Method: other: unknown
GLP: no
Remark: Solidification point
Source: Unichema Chemie GmbH Emmerich

(3)

Value: 31.2 - 31.6 degree C
Decomposition: no
Sublimation: no
Method: other: unknown
Source: Unichema Chemie GmbH Emmerich

(4)

Value: 31.5 degree C
Decomposition: no
Sublimation: no
Method: other: not known
Source: Unichema Chemie GmbH Emmerich

(5)

2.2 Boiling Point

Value: 268 - 270 degree C at 1000 hPa
Decomposition: no
Source: Unichema Chemie GmbH Emmerich

(6)

Value: 270 degree C at 1013 hPa
Decomposition: no
Source: Unichema Chemie GmbH Emmerich

(7)

Value: 270.6 degree C at 1013.33 hPa
Decomposition: no
Remark:

b.p.	(hPa=mbar)	b.p.	(hPa=mbar)
55.0	0.0133	174.6	42.67
79.0	0.133	178.7	53.33
99.6	0.67	191.3	85.33
110.3	1.33	202.0	133
121.1	2.66	209.8	170.67
132.7	5.33	222.7	266
137.0	6.67	230.6	341.33
145.5	10.67	246.7	522
148.7	13.33	254.9	682.33
159.4	21.33	261.3	800
163.3	26.67	270.6	1013.33

Source: Unichema Chemie GmbH Emmerich

(8)

Value: 268.4 degree C at 1013.33 hPa
Decomposition: no
Remark: b.p. (hPa=mbar)
125.0 (1.33)
142.0 (6.65)
152.2 (13.3)
165.0 (26.6)
179.9 (53.2)
189.8 (79.8)
200.0 (133)
217.1 (266)
240.3 (532)
Source: Unichema Chemie GmbH Emmerich
(9) (10) (11)

2.3 Density

Type: density
Value: = .92 g/cm3 at 20 degree C
Source: Henkel KGaA Duesseldorf
(12)

Type: relative density
Value: 1.0176 g/cm3 at 25 degree C
Remark:

Rel. Density	(gr C)	Rel. Density	(gr C)
1.0266	(15)	0.8618	(70)
1.0176	(25)	0.8583	(75)
0.8884	(35)	0.8531	(80)
0.8858	(40)	0.8372	(100)
0.8773	(50)	0.8056	(140)
0.8701	(60)		

Source: Unichema Chemie GmbH Emmerich
(13)

Type: bulk density
Value: ca. 850 kg/m3 at 75 degree C
Source: Unichema Chemie GmbH Emmerich
(7)

2.3.1 Granulometry

-

2.4 Vapour Pressure

Value: < 1 hPa at 20 degree C
Source: Unichema Chemie GmbH Emmerich
(7)

Value: < .013 hPa at 25 degree C

Remark:

T (°C)	v.p.(hPa)	T (°C).	v.p.(hPa)
55.0	0.0133	174.6	42.67
79.0	0.133	178.7	53.33
99.6	0.67	191.3	85.33
110.3	1.33	202.0	133
121.1	2.66	209.8	170.67
132.7	5.33	222.7	266
137.0	6.67	230.6	341.33
145.5	10.67	246.7	522
148.7	13.33	254.9	682.33
159.4	21.33	261.3	800
163.3	26.67	270.6	1013.33

Source: Unichema Chemie GmbH Emmerich

(8)

Value: 1.3 hPa at 125 degree C

Remark:

vap.pres. (hPa)	temp (°C)
1.33	125.0
6.65	142.0
13.3	152.2
26.6	165.0
53.2	179.9
79.8	189.8
133	200.0
266	217.1
532	240.3

Source: Unichema Chemie GmbH Emmerich

(14)

Value: = 1.33 hPa at 125 degree C
Source: Henkel KGaA Duesseldorf
Test substance: decanoic acid

(15)

Value: 1.33 hPa at 125 degree C
Source: Unichema Chemie GmbH Emmerich

(6)

2.5 Partition Coefficient

log Pow: = 4.09
Method: other (measured): Method not stated
Year:
Source: Henkel KGaA Duesseldorf
Test substance: decanoic acid

(16)

log Pow: 4.1
Method:
Year:
Source: Unichema Chemie GmbH Emmerich

(7)

2.6.1 Water Solubility

Value: .15 g/l at 20 degree C
Qualitative: of very low solubility
Remark: solubility (g/l) (degree C)

solubility (g/l)	(degree C)
0.095	0
0.15	20
0.18	30
0.23	45
0.27	60

Soluble in many organic solvents
Source: Unichema Chemie GmbH Emmerich

(17)

Value: at 20 degree C
Qualitative: not soluble
Source: Henkel KGaA Duesseldorf

(12)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: = 135 degree C
Type: open cup
Method: other: DIN ISO 2592
Year:
Source: Henkel KGaA Duesseldorf

(12)

Value: 145 degree C
Type: open cup
Method:
Year:
Source: Unichema Chemie GmbH Emmerich

(18)

Value: 150 degree C
Type: open cup
Method: other: ISO 2592-1973 (Cleveland Open Cup)
Year:
GLP: no data
Source: Unichema Chemie GmbH Emmerich

(7)

2.8 Auto Flammability

Value:
Remark: Based on data of similar substances, it is not expected thatdecanoic acid has not an extremely low self ignition temperature.
not determined
Source: Unichema Chemie GmbH Emmerich

2.9 Flammability

Result: non flammable
Remark: On account of the molecular and the chemical structure it isnot to be expected that decanoic acid:
- will produce flammable gasses if in contact with water
- will show sponteneous ignition in cntact with inert material and intense contact with air. (i.e. pyrophoric properties).

Source: Unichema Chemie GmbH Emmerich

2.10 Explosive Properties

Result: not explosive
Remark: On account of the molecular and the chemical structure of decanoic acid, no explosive properties are to be expected.
Source: Unichema Chemie GmbH Emmerich

2.11 Oxidizing Properties

Result: no oxidizing properties
Remark: On account of the molecular and the chemical structure of decanoic acid, no oxidizing properties are to be expected.
Source: Unichema Chemie GmbH Emmerich

2.12 Additional Remarks

Remark: Viscosity (40°C) 5.37 mPa.s
Viscosity (100°C) 1.69 mPa.s
Source: Unichema Chemie GmbH Emmerich
(19)

Remark: Surface tension (20°C) 28.2 mN.m
Source: Unichema Chemie GmbH Emmerich
(19)

Remark: Specific grafity 0.886 at 40/4°C
Source: Unichema Chemie GmbH Emmerich
(6)

3.1.1 Photodegradation

-

3.1.2 Stability in Water

-

3.1.3 Stability in Soil

-

3.2 Monitoring Data (Environment)

-

3.3.1 Transport between Environmental Compartments

-

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

-

3.5 Biodegradation

Type: aerobic
Inoculum: other: sewage treatment plant effluent/biological stage
Concentration: 2 mg/l
Degradation: 100 - 71 % after 30 day
Result: readily biodegradable
Method: Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year: **GLP:**
Test substance: other TS
Remark: Original experimental data: ungenüg. Rest O2 5ppm Prüfmuster als Natriumsalz bewertet..
Source: Henkel KGaA Duesseldorf
Test condition: #1: 2 mg/l referring to Active Substance: 100% with parameter % BSB/CSB
#2: 5 mg/l referring to Active Substance: 71% with parameter % BSB/CSB
Test substance: Analogy; data taken from CASRN 124-07-2 <Octanoic acid>, Active Matter > 100 %.

(20) (21) (22)

Type: aerobic
Inoculum: activated sludge
Method:
Year: **GLP:**
Test substance:
Source: Unichema Chemie GmbH Emmerich

Type:
Inoculum: predominantly domestic sewage, adapted
Degradation: = 60.9 % after 5 day
Method: other: 5 day BOD according to "Standard Methods for the Examination of Water & Wastewater", American Public Health Association (1980)
Year: 1980 **GLP:**
Test substance:
Remark: parameter: BOD5 [mmole/mmole substrate]/BOD theoretical
Source: Henkel KGaA Duesseldorf
Test condition: 21 +/- 3 degr. C; microbial culture from domestic sewage adapted to test substance prior to test
Test substance: Chain length: C10

(23)

Type:
Inoculum: activated sludge
Concentration: 500 mg/l related to Test substance
Degradation: = 23.4 % after 1 day
Method: other: Warburg respirometer test
Year: **GLP:**
Test substance:
Remark: parameter: oxygen uptake
Source: Henkel KGaA Duesseldorf
Test substance: Chain length: C10

(24)

Type:
Inoculum:
Result: readily biodegradable
Kinetic:
6 hour(s) 10.9 %
12 hour(s) 18.9 %
24 hour(s) 23.4 %
Method:
Year: **GLP:**
Test substance:
Remark: Based on data for structural similar substances
Waste water treatment: percentage of ThOD
Source: Unichema Chemie GmbH Emmerich

(7) (6)

3.6 BOD5, COD or BOD5/COD Ratio

R A T I O B O D 5 / C O D

BOD5/COD: .106

Remark: BOD5: 9% of ThOD
COD : 85% of ThOD
Source: Unichema Chemie GmbH Emmerich

(6)

3.7 Bioaccumulation

Species:
Exposure period:
Concentration:
BCF:
Elimination:
Method:
Year: **GLP:**
Test substance:
Remark: log Poct=4.09
Source: Unichema Chemie GmbH Emmerich
(6)

3.8 Additional Remarks

Remark: Odor treshold: detection 10.0 mg/kg
Source: Unichema Chemie GmbH Emmerich
(6)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: semistatic
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 54
Method: other
Year: **GLP:**
Test substance:
Source: Henkel KGaA Duesseldorf
Test condition: freshwater (renewal every 24 h); 25 +- 2 degr. C; pH 7.2; concentration of test substance determined by HPLC
Test substance: Chain length: C10 (sodium salt was tested)

(25)

Type:
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
LC0: 30
LC50: 95
LC100: 300
Method: other: DIN 38412, Teil 15 (Golden orfe, acute toxicity test)
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Related to: Test substance
Vorbehandlung: Direkteinwaage + Ultraturrax
Source: Henkel KGaA Duesseldorf
Test substance: Active Matter = 100 %

(26) (27)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 31
Method: other: Seawater test
Year: **GLP:**
Test substance:
Remark: Oryzias is not a marine species, but can be gradually adapted to seawater.
Source: Henkel KGaA Duesseldorf
Test condition: salinity: 30 ppt; 25 +/- 2 degr. C; pH 8.2; concentration of test substance determined by HPLC
Test substance: Chain length: C10

(25)

Type: other
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: chemical is to insoluble in water to be toxic
Source: Unichema Chemie GmbH Emmerich

(6)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Artemia salina (Crustacea)
Exposure period: 16 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: = 36
Method: other: According to Harwig & Scott, Appl. Microbiol. 21 (1971), 1011 ff.
Year: 1971 **GLP:**
Test substance:
Source: Henkel KGaA Duesseldorf
Test substance: Chain length: C10

(28)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:**
EC50: = 65
Method: other: AFNOR T.90301 (1974). Determination de l'inhibition de la mobilite de Daphnia magna Straus.
Year: 1974 **GLP:**
Test substance:
Source: Henkel KGaA Duesseldorf
Test substance: Chain length: C10 (sodium salt was tested)

(29)

Species: other aquatic arthropod: Hyale plumulosa (gammarus)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 41
Method: other
Year: **GLP:**
Test substance:
Remark: parameter: mortality
Source: Henkel KGaA Duesseldorf
Test condition: salinity: 25 ppt; 25 +/- 2 degr. C; pH 8.2; concentration of test substance determined by HPLC

(25)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: Nitzschia closterium (marine diatom)
Endpoint: other: cell growth
Exposure period: 72 hour(s)
Unit: mmol/l **Analytical monitoring:**
EC50: = .002
Method: other
Year: **GLP:**
Test substance:
Remark: 0.002 mmol/l = 0.3 mg/l
parameter: cell growth measured spectrophotometrically
Source: Henkel KGaA Duesseldorf
Test condition: natural seawater
Test substance: Chain length: C10

(30)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Photobacterium phosphoreum (Bacteria)
Exposure period: 25 minute(s)
Unit: µmol/l **Analytical monitoring:** no data
EC50: = 47.1 - 57.5
Method: other: Microtox
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Source: Henkel KGaA Duesseldorf

(31)

Type: aquatic
Species: other bacteria: Bifidobacterium bifido
Exposure period:
Unit: mmol/l **Analytical monitoring:** no data
EC50: = 50
Method: other: Growth Inhibition-Test
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: ED50 means value of added lipid concentration (mM) producing 50 % bacterial growth inhibition.
Source: Henkel KGaA Duesseldorf

(32)

Type:
Species: Bacillus subtilis (Bacteria)
Exposure period: 60 minute(s)
Unit: mmol/l **Analytical monitoring:**
EC50: = .25
Method: other
Year: **GLP:**
Test substance:
Remark: 0.25 mmol/l = 43.1 mg/l
parameter: inhibition of rate of duplication
Source: Henkel KGaA Duesseldorf
Test condition: complex medium; 37 degr. C; ethanol as solvent for test substance (final conc. < 1 %)
Test substance: Chain length: C10

(33)

Type:
Species: Pseudomonas putida (Bacteria)
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:**
EC0: 3000
EC10 : 10000
Method: other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Method: Method conforms with OECD Guide-line 209
Remark: Direkteinwaage + Ultraturrax.
Related to: Test substance
Source: Henkel KGaA Duesseldorf
Test substance: Active Matter = 100 %

(34) (27)

Type:
Species: other bacteria: Bacillus megaterium
Exposure period: 24 hour(s)
Unit: mmol/l **Analytical monitoring:**
MIC : = 1
Method: other
Year: **GLP:**
Test substance:
Remark: 1 mmol/l = 172.26 mg/l
MIC = minimum inhibitory concentration
parameter: growth determined visually or by plate count technique
Source: Henkel KGaA Duesseldorf
Test condition: exposure to test substance for 24 h at 25 degr. C in nutrient broth; ethanol as solvent for test substance
Test substance: Chain length: C10

(35)

Type:
Species: other bacteria: Methanothrix sp.
Exposure period: 24 hour(s)
Unit: mmol/l **Analytical monitoring:**
EC50: = 5.9
MIC : = 2.6
Method: other
Year: **GLP:**
Test substance:
Remark: 5.9 mmol/l = 1016 mg/l
2.6 mmol/l = 448 mg/l
MIC = minimum inhibitory concentration
parameter: inhibition of acetoclastic methanogenic activity
Source: Henkel KGaA Duesseldorf
Test condition: Upflow anaerobic sludge bed rector (predominant methanogen in sludge: Methanothrix); 30 degr. C; pH 7; concentration of test substance determined by GC
Test substance: Chain length: C10

(36)

Type:
Species: other bacteria: Streptococcus mutans
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:**
MIC : > 100
Method: other
Year: **GLP:**
Test substance:
Remark: Determination of MIC (minimum inhibitory concentration) by visually judging bacterial growth
Source: Henkel KGaA Duesseldorf
Test condition: T = 37 degr. C; methanol as solvent (concentration not stated)
Test substance: Chain length: C10

(37)

Type:
Species: other bacteria: Vibrio parahaemolyticus
Exposure period: 9 hour(s)
Unit: mg/l **Analytical monitoring:**
MIC : = 60
Method: other
Year: **GLP:**
Test substance:
Remark: MIC = minimum inhibitory concentration
parameter: arithmetic difference between percentage transmittance (620 nm) of control & test cultures
Source: Henkel KGaA Duesseldorf
Test condition: 30 degr. C; cultures in complex medium; ethanol as solvent (values corrected for control containing only ethanol)
Test substance: Chain length: C10

(38)

Type:
Species: aerobic microorganisms
Exposure period:
Unit: mmol/l **Analytical monitoring:**
EC50: = 13.8
Method: other
Year: **GLP:**
Test substance:
Remark: 13.8 mmol/l = 2 377 mg/l
parameter: reduction in heat flux (determined with flow microcalorimeter)
Source: Henkel KGaA Duesseldorf
Test condition: 25 degr. C; origin and composition of microbial culture not specified
Test substance: Chain length: C10 (potassium salt was tested)

(39)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

-

4.5.2 Chronic Toxicity to Aquatic Invertebrates

-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species: Panagrellus redivivus (Worm (Nematoda), soil dwelling)
Endpoint: other: immobilization
Exposure period: 1 hour(s)
Unit: other: ppm
ED95 : = 156
Method:
Year: **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: ED95 means the concentration that immobilizes 95% of the test nematodes within 1 hour.
Source: Henkel KGaA Duesseldorf

(40)

4.6.2 Toxicity to Terrestrial Plants

-

4.6.3 Toxicity to other Non–Mamm. Terrestrial Species

-

4.7 Biological Effects Monitoring

-

4.8 Biotransformation and Kinetics

-

4.9 Additional Remarks

-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 10000 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: A dose of 4.6 g/kg bw or more caused excessive salivation and diarrhoe. At 10000 mg/kg bw, discharge from eyes and nose, some reduction of neuromuscular control and central nervous system depression were seen. No gross abnormalities were seen in lungs, kidneys, digestive tract and adrenals.
Source: Henkel KGaA Duesseldorf

(41) (42)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3320 mg/kg bw
Method:
Year: **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Henkel KGaA Duesseldorf

(43)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 10 mg/kg bw
Method: other
Year: 1976 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: The method used was as specified in the Regulations for the Enforcement of the Federal Hazardous Substances Act (Revised, Federal Register, Sept. 17, 1964) and Title 49 Department of Transportation Code of Federal Regulation, Section 173, 240 (Federal Register, Feb 12, 1973).
Source: Unichema Chemie GmbH Emmerich

(44)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3730 mg/kg bw
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Unichema Chemie GmbH Emmerich
Test substance: Mixed isomer of decanoic acid

(45)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: 15800 mg/kg bw
Method: other: 10 animals used
Year: 1975 **GLP:** no data
Test substance: other TS
Source: Unichema Chemie GmbH Emmerich
Test substance: 5% decanoic acid in 40% w/w ethanol

(46)

5.1.2 Acute Inhalation Toxicity

Type: other
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 8 hour(s)
Value:
Method: other
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Rats were exposed to saturated vapours of the mixed isomer of decanoic acid. The maximum exposure time without any deaths occuring was 8 hours.
Source: Unichema Chemie GmbH Emmerich

(45)

5.1.3 Acute Dermal Toxicity

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: Limit-Test
Source: Henkel KGaA Duesseldorf

(47)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value:
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: The dermal LD50 is given as 1.77ml/kg.
Source: Unichema Chemie GmbH Emmerich
Test substance: Mixed isomer of decanoic acid

(45)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Unichema Chemie GmbH Emmerich

(45)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 129 mg/kg bw
Method:
Year: **GLP:**
Test substance:
Remark: Doses approaching the LD50 caused convulsions and collapse.
Source: Henkel KGaA Duesseldorf

(47)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.v.
Value: = 129 mg/kg bw
Method:
Year: 1992 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Source: Unichema Chemie GmbH Emmerich

(48)

Type: LC100
Species: other
Sex:
Number of Animals:
Vehicle:
Route of admin.: other
Exposure time: 24 hour(s)
Value: <= 10 mg/l
Method: See remarks
Year: 1991 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: The toxicities of saturated straight chain fatty acids (including decanoic acid) were evaluated using rice bloodworm larvae. Mortality was assessed after 24 hours exposure to 1, 10 or 50mg/l. Four groups of ten larvae were used for each test material.

Decanoic acid caused 100% mortality at 10 or 50mg/l; at 1mg/l it caused 12-15% mortality.
Source: Unichema Chemie GmbH Emmerich

(49)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other
Year: **GLP:**
Test substance:
Remark: Covered contact for 4-24 hr with neat decanoic acid proved moderately to severely irritating to intact and abraded skin.
Kontaktzeit 4-24 h
Source: Henkel KGaA Duesseldorf

(41)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method:
Year: 1992 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Exposure to 500mg for 24 hours caused moderate irritation.
Source: Unichema Chemie GmbH Emmerich

(50)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: highly irritating
EC classificat.:
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Undiluted decanoic acid was applied to intact and abraded rabbit skin under occlusion for 24 hours. Reactions were moderate-severe.

Source: Unichema Chemie GmbH Emmerich

(45)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other: 3 rabbits used; erythema and edema evaluated
Year: 1969 **GLP:** no data
Test substance: other TS
Source: Unichema Chemie GmbH Emmerich
Test substance: 5% decanoic acid in water, ethanol or a combination of the two

(51)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other
Year: **GLP:**
Test substance:
Remark: 17.2 %ig, okklusiv, Kontaktzeit 24 h
Source: Henkel KGaA Duesseldorf

(41)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other
Year: **GLP:**
Test substance:
Remark: 1 %ig, okklusiv, Kontaktzeit 24 h
Source: Henkel KGaA Duesseldorf

(41)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other
Year: **GLP:**
Test substance:
Remark: 8.6 %, okklusiv, Kontaktzeit 24 h, wiederholt
Daily applications of 8.6 % decanoic acid in propanol to ten subjects caused irritation with reddening in three after 2 days and in seven after 8 days.
Source: Henkel KGaA Duesseldorf

(41)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.: irritating
Method: other
Year: 1993 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Ten healthy male volunteers were exposed to 1.0M solutions of various fatty acids (C3-C18) under occlusion for 10 days.C8-C11 produced an irritant response in all ten subjects by the end of the test; no irritation had been evident on day 1of the test. Therefore these four fatty acids (including decanoic acid) showed distinct cumulative irritation potential, but no acute irritation potential.
Source: Unichema Chemie GmbH Emmerich

(52)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method: other
Year: 1994 **GLP:** yes
Test substance: other TS
Remark: Prifrac 2910 was applied undiluted under occlusion to human

skin for up to four hours. The test method was similar to the standard rabbit skin irritation test. The results were similar to those obtained with 20% sodium dodecyl sulphate (a standard irritant) on the same volunteers.

Source: Unichema Chemie GmbH Emmerich
Test substance: Prifrac 2910, a mixture of 54% caprylic acid and 44.5% capric (decanoic) acid.

(53)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: not irritating
EC classificat.:
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: 1% decanoic acid in petrolatum caused no irritation in a 48 hour occluded patch test.
Source: Unichema Chemie GmbH Emmerich

(54)

Species: human
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.:
Method:
Year: 1979 **GLP:**
Test substance: as prescribed by 1.1 - 1.4
Remark: Solutions of decanoic acid were applied daily to ten male volunteers for up to 10 days. 0.5M capric acid caused an erythematous response in 7/10 volunteers within 8 days; 1.0Mdecamoic acid caused a response in all 10 volunteers within 8 days.
Source: Unichema Chemie GmbH Emmerich

(55)

Species: other
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: irritating
EC classificat.: irritating
Method: In-vitro test
Year: 1993 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Fatty acids of varying chain lengths C3-C18 were used in this study. Previous human skin data indicated that C8-C14 were the most irritant (cumulative irritancy). The in vitrodata were compared with previous in vivo data.

The Primary Dermal Irritation Index (PDII) for decanoic acidwas 0.81, or 0.75, depending on the in vitro protocol used. The manufacturers of Skintex recommend a PDII cut-off of 0.35, therefore the in vitro method correctly identified decanoic acid as irritant. However, the Skintex method onlyhad a sensitivity of 83% and a specificity of 50% overall. This may be due either to the Skintex system not being able to predict cumulative irritants, and/or to difficulties in defining the appropriate human cut-off point for irritancy.
Source: Unichema Chemie GmbH Emmerich
(56)

Species:
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: corrosive
EC classificat.: corrosive (causes burns)
Method: other
Year: 1976 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Method as given in section 5.1.1, record 1. Animals (species not defined) were exposed to decanoic acid under a 24 hour patch. The primary skin irritation index was 4.60.

In a 4 hour skin corrosivity test decanoic acid produced blanching of one site and necrosis of one site at the 4 hourreading. At the 24 and 48 hour readings, entire or spotted coriaceousness was observed at some sites.
Source: Unichema Chemie GmbH Emmerich
(57)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: highly irritating
EC classificat.:
Method: other
Year: **GLP:**
Test substance:
Remark: 0.1 ml / Tier; Dauerkontakt
Instillation of neat material caused corneal clouding and moderate inflammation of the conjunctivae and iris.
Source: Henkel KGaA Duesseldorf

(41)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other
Year: 1976 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: The method used id referenced in section 5.1.1, record 1.
Decanoic acid caused corneal opacity and moderate conjunctivitis which did not subside in 72 hours.
Source: Unichema Chemie GmbH Emmerich

(57)

5.3 Sensitization

Type: Buehler Test
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other
Year: 1975 **GLP:** no data
Test substance: other TS
Remark: One test group (20 animals) and one control group (10 animals) were used. For induction, a closed patch was applied for 6 hour once a week for three weeks.
Two weeks later, a challenge patch was applied for 6 hours (5% decanoic acid in acetone). Animals were examined at 24 and 48 hours.

Result showed no sensitization in either group (0/20 and 0/10 for test and control groups, respectively).

Source: Unichema Chemie GmbH Emmerich
Test substance: 5% decanoic acid in 40% w/w ethanol

(58)

Type: other
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other
Year: 1979 **GLP:**
Test substance:
Remark: A human maximisation test was carried out on 28 volunteers. 1% concentration (described as RIFM no. 76-35) caused no sensitization reactions.
Source: Unichema Chemie GmbH Emmerich

(55)

Type:
Species: human
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other: according to Kligman & Epstein
Year: **GLP:**
Test substance:
Remark: Five 48 hr covered applications of 1 % decanoic acid in petrolatum were made over a 10 day period in 28 volunteers. None of them gave positive reactions when challenged 10-14 days after the induction phase with a final 48 hr closed patch test using 1 % in petrolatum.
Source: Henkel KGaA Duesseldorf

(59) (47)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** no data
Strain: no data
Route of admin.: oral feed
Exposure period: 150 Tage
Frequency of treatment: Dauerangebot
Post. obs. period: keine Angabe
Doses: 10 % (ca. 5 g/kg/Tag)
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Result: Ten rats fed 10 % dietary decanoic acid did not develop gross changes of the forestomach or glandular stomach.
Source: Henkel KGaA Duesseldorf

(41)

Species: rat **Sex:** male/female
Strain: no data
Route of admin.: oral feed
Exposure period: 47 Wochen
Frequency of treatment: Dauerangebot
Post. obs. period: keine Angabe
Doses: ca. 2.5 g Decansaeure + 7.4 g Octansaeure/kg/Tag Triglycerid
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Result: Mortality, growth, organ weights and the cellular structure of the liver and instestine were normal in groups of 15 rats each sex fed a diet providing decanoic acid as triglyceride.
Source: Henkel KGaA Duesseldorf

(41)

Species: rat **Sex:** male/female
Strain: Sprague-Dawley
Route of admin.: oral feed
Exposure period: 91 days
Frequency of treatment: Daily feed
Post. obs. period: None
Doses: 0, 5.23, 10.23 and 15.00% w/w in diet
Control Group: yes
NOAEL: > 13200 mg/kg bw
Method: other
Year: 1993 **GLP:** no data
Test substance: other TS
Remark: Although it is not positively stated, it is anticipated thatthe work was conducted to GLP standards.
Groups of 25 male and 25 female weanling rats were fed diets(ad lib.) containing one of the following:

- 12.14% w/w corn oil
- 11.21% MCT oil
- 5.23% w/w caprenin
- 10.23% w/w caprenin
- 15.00% w/w caprenin

Corn oil was added to all diets to provide essential fatty acids; the diets were balanced for fat, protein and carbohydrate. It was also intended to balance calorie intake (caprenin is a relatively poor energy source due to low absorption of the behenic acid component), but the results indicated that caprenin did not provide 5kcal/g energy for all dose groups (lower in the high dose group, due to high level of behenic acid).

Survival, clinical signs, body weight, feed consumption, feed efficiency, organ weights, organ-to-body weight/brain weight ratios, haematological values and clinical chemistry parameters were evaluated in all groups. Histopathology of a full range of tissues was evaluated in the corn oil and MCT oil control groups, as well as the high dose caprenin group. An additional 5 rats/sex/group were included to determine whether storage of C22:0 occured in the heart, liver or peri-renal fat.

Result: No significant differences were observed in body weight gainwith the balanced caloric diets, although feed conversion efficiency was reduced in the high-dose caprenin group. No significant adverse effects from ingestion of caprenin were observed, nor were significant amounts of C22:0 present in selected fat depots.

Some effects associated with caprenin were observed, but were not considered a significant toxicological effect. Forexample, lower liver-to-body weight ratios were observed in male rats fed caprenin, and lower absolute liver weights were observed in female rats fed caprenin. This was thoughtto be due to the reduced amount of fat depositied in the livers of rats fed caprenin diets. Female mid- and high-dose animals significantly higher serum ALT values. This was thought to be due to the imbalance of digestible calories. Rats fed caprenin also showed higher colon weights (absolute and relative). This was thought to be related to the poor absorption of behenic acid, and consequently a greater fecal weight, resulting in colon enlargement. The authors concluded that the above changes were not a toxicological response, but an adaption to the high level of behenic acid in the diet.

Source: Unichema Chemie GmbH Emmerich

Test substance: Caprenin, a triglyceride comprising mainly of caprylic (C8:0), capric (C10:0) and behenic (C22:0) acids.

(60)

Species: rat **Sex:** male/female

Strain: Wistar

Route of admin.: oral feed

Exposure period: 47 weeks

Frequency of treatment: Daily feed

Post. obs. period: None

Doses: 40% MCT in diet

Control Group:

Method: other

Year: 1972 **GLP:** no

Test substance: other TS

Remark: 15 male and 15 female rats were fed the triglyceride diet for 47 weeks. Blood samples, weight gain and fecal samples were taken/analysed during the experimental phase. Organ weights were taken at necropsy, and limited microscopic analysis was performed. Various organs and the carcass wereanalysed for fat content.

Result: No adverse effects were observed. Fat deposition was lower than might be expected on normal fat diets.

Source: Unichema Chemie GmbH Emmerich

Test substance: The diet contained 40% medium chain triglyceride (MCT); the MCT contained 21% decanoic acid.

(61)

Species: rat **Sex:**
Strain:
Route of admin.: oral feed
Exposure period: 150 days
Frequency of treatment: Daily feed
Post. obs. period: None
Doses: 10%
Control Group:
Method:
Year: 1979 **GLP:** no
Test substance: as prescribed by 1.1 - 1.4
Remark: No gastric lesions were observed in this study. No other details are given in the summary presented.
Source: Unichema Chemie GmbH Emmerich

(45)

Species: dog **Sex:** no data
Strain: no data
Route of admin.: oral feed
Exposure period: 102 Tage
Frequency of treatment: Dauerangebot
Post. obs. period: keine Angabe
Doses: ca. 4.4 g/kg/Tag
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Result: An unstated number of test animals showed no changes in organ weights, structure and function of liver or kidney, or electrical activity of the heart.
Source: Henkel KGaA Duesseldorf

(41)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium (keine weiteren Angaben)
Concentration:
Metabolic activation: no data
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: Henkel KGaA Duesseldorf

(41) (62)

Type: Ames test
System of testing: Salmonella typhimurium (TA97, TA98, TA100, TA1535 & TA1537)
Concentration: 0-666ug/plate
Metabolic activation: with and without
Result: negative
Method:
Year: 1988 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Although it is not specifically stated, it is assumed that these studies were conducted to a standard protocol and GLP (the studies were conducted in conjunction with the NationalToxicology Program, USA).
Source: Unichema Chemie GmbH Emmerich

(63)

Type: Escherichia coli reverse mutation assay
System of testing: E.coli
Concentration:
Metabolic activation: without
Result: negative
Method: other
Year: 1958 **GLP:** no data
Test substance: as prescribed by 1.1 - 1.4
Remark: Test materials are applied to agar plates innoculated with various concentrations of E. coli strain Sd-4-73 (streptomycin dependent). The test materials are either applied directly to the agar, or on filter paper discs.

Decanoic acid was reported as having no mutagenic activity.
Source: Unichema Chemie GmbH Emmerich

(64)

Type:
System of testing: E. coli (keine weiteren Angaben)
Concentration:
Metabolic activation: no data
Result: negative
Method:
Year: **GLP:**
Test substance:
Source: Henkel KGaA Duesseldorf

(41)

5.6 Genetic Toxicity 'in Vivo'

-

5.7 Carcinogenicity

-

5.8 Toxicity to Reproduction

Type: Two generation study
Species: rat **Sex:** male/female
Strain: other
Route of admin.: oral feed
Exposure Period: 3 weeks before mating
Frequency of treatment: Daily feed
Premating Exposure Period
male: 3 weeks
female: 3 weeks
Duration of test:
Doses:
Control Group: yes
Method: other
Year: 1972 **GLP:** no
Test substance: other TS
Remark: 12 week old McCollum-Wisconsin rats were fed diets containing MCT (unspecified level). Three weeks later the rats were mated. The F1 offspring were fed on normal diet for 12 weeks, and then fed the same MCT diet, and mated 3 weeks later.
Result: There were no adverse effects on the F1 litter size or birthweight. Milk secretion of the F1 rats was significantly reduced. There was also a higher mortality (20-22%) during lactation for the F2 group fed the MCT diet.
Source: Unichema Chemie GmbH Emmerich
Test substance: MCT (medium chain triglyceride) contained 25% decanoic acid.
(65)

Type: other
Species: rat **Sex:** male/female
Strain: no data
Route of admin.: oral feed
Exposure Period: 3 Wochen vor der Paarung, waehrend der Traechtigkeit und Laktation, Nachwuchsbehandlung
Frequency of treatment: Dauerangebot
Duration of test:
Doses: ca. 2.5 Decansaeure + 4.7 Octansaeure g/kg/Tag als Triglycerid
Control Group: no data specified
Method:
Year: **GLP:**
Test substance:
Remark: Nachbeobachtung: keine Angabe
Result: A diet providing about 2.5 g decanoic acid and about 7.4 g octanoic acid/kg bw/day (as triglycerides) was fed to an unspecified number of male and female rats from 3 wk prior to mating, throughout pregnancy and lactation and to the weaned offspring for 15 wk prior to their mating. Their was no effect on pup birth weight or litter size in either generation. Females of the second generation produced milk of lower nutritional quality and quantity, and the investigators suggested that this was responsible for the increased mortality of their offspring.
Source: Henkel KGaA Duesseldorf

(41)

Type: other
Species: other **Sex:**
Strain:
Route of admin.:
Exposure Period:
Frequency of treatment:
Duration of test:
Doses:
Control Group:
Method:
Year: **GLP:**
Test substance:
Remark: Decanoic acid was highly toxicto the eggs of the amphibian Triturus helveticus. A saturated (0.1M) solution caused cytolysis within one hour.
Source: Unichema Chemie GmbH Emmerich

(55)

5.9 Developmental Toxicity/Teratogenicity

-

5.10 Other Relevant Information

Type: adsorption
Remark: Skin permeation rates were measured in vitro using human skin samples. Six model compounds of diverse physicochemical properties were dissolved in propylene glycol, and the permeation rates studied in the presence andabsence of various fatty acids (including decanoic and neodecanoic acid).

Both decanoic and neodecanoic acid increased the skin diffusivity of four of the six model compounds, but only decanoic acid increased the permeation rate of propylene glycol.

Overall the studies demonstrated that permeation rates couldbe increased by improved drug solubilization in the vehicle,increased partitioning, increased solvent penetration, and barrier disruption. The relative contributions of the mechanisms vary with the drug, the adjuvant and the vehicle.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid and neodecanoic acid (branched C10 fatty acid).

(66)

Type: adsorption
Remark: The enhancing action of decanoic acid on the intestinal absorption of phenosulphonphthalein (PSP) was studied in rats. Decanoic acid and two hydroxy derivatives enhanced PSP absorption to varying degrees; PSP was no longer absorbed once the enhancer had been completely absorbed. Absorption enhancement correlated with the ability to sequester calcium ions.
Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(67)

Type: adsorption
Remark: The influenec of triglyceride structure on intestinal absorption was investigated. Thet triglycerides were composed of octanoic (C8), decanoic (C10) and linoleic (C18:2) acids (either as a structured oil, with the C8 and C10 at the sn-1 and sn-3 positions, or as a randomised oil, with the three acids in a random distribution). Absorbtion of the three acids varied; absorbtion of the C18:2 was highest from the structured oil, when it occupied the sn-2 position. Absorption of the two shorter chain fatty acids was highest from the randomised oil, when both acids occupied the sn-2 position approximately 33% of the time.
Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(68)

Type: adsorption
Remark: The in vitro human skin permeation rate of an analgesic (buprenorphine) was increased by a factor of 3.5 by the addition of 0.5% decanoic acid.
Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(69)

Type: adsorption
Remark: Sodium caprate increased the epithelial permeability of PEG 4000 by 3.5 times in cultures Caco-2 cells. This correlatedwith previous in vivo experiments with rat jejunum and colonin situ. PEG 4000 is poorly absorbed on its own. The absorption enhancing effect of sodium caprate was unchanged in the absence of mucosal Ca2+, suggesting that the mode of action does not depend on Ca2+ chelation.
Source: Unichema Chemie GmbH Emmerich
Test substance: Sodium caprate

(70)

Type: adsorption
Remark: The rate of intestinal absorption and hepatic uptake of medium chain fatty acids (MCFA) was investigated in 6 pigs. The pigs were fitted with a permanent fistula in the duodenum, and catheters in the portal vein, carotid artery and hepatic vein.

Decanoic acid (esterified with octanoic acid) was infused into the duodenum for 1 hour. Regular blood samples were taken over 12 hours and analysed for non-esterified decanoicacid content.

Decanoic acid levels in portal vein blood rose sharply afterthe beginning of the infusion (confirming data previously reported for dogs and rats), and showed a bi-phasic time course with two maximum values (at 15 minutes and 75-90 minutes).

54% of the decanoic acid was recovered in portal blood samples.

The amounts of non-esterified MCFA taken up per hour by the liver were close to those absorbed from the gut via the portal vein, showing that the liver is the main site of MCFAmetabolism in pigs.

Source: Unichema Chemie GmbH Emmerich

Test substance: Decanoic acid, esterified with octanoic acid as medium-chaintriacylglycerols

(71)

Type: adsorption

Remark: The influence of pancreatic enzyme secretion on the intestinal absorption of medium-chain fatty acids (MCFA) wasinvestigated in 3 pigs. The pancreatic ducts were ligated (so producing exocrine pancreatic deficiency) and fitted with a permanent fistula, and catheters fitted in the portalvein and carotid artery. The decanoic acid tricylglycerol mixture was infused into the duodenum for 1 hour. Blood samples were taken over 8 hours and analysed for non-esterified decanoic acid content.

Decanoic acid level increased slowly after the start of the infusion, reaching a maximum after 90-120 minutes. This contrasts with previous studies (see record 13), where healthy pigs reached a maximum blood concentration after 15 minutes. This indicates that pancreatic lipase activity is not the pathway for de-esterification of MCFA.

27% of the decanoic acid was recovered from the portal bloodflow. This is lower than seen previously, but confirms thatmore than one pathway is involved as decanoic acid production was not completely suppressed.

Source: Unichema Chemie GmbH Emmerich

Test substance: Decanoic acid, esterified with octanoic acid as medium-chaintriacylglycerols.

(72)

Type: adsorption

Remark: 14C-labelled fatty acids (including 240mg decanoic acid) were fed by intubation into lactating rabbits. The animals were killed 24 hours later, and the mammary gland lipids were analysed.

Decanoic acid was extensively metabolised. Resynthesis after degradation to C2 units led to uniform alternate labelling in the C2-C10 acids, whereas C12-C18 acids had an excess of 14C at the carboxyl end. Acids formed by beta-oxidation down to C12 (but not below) were also presentin the mammary gland lipids.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(73)

Type: adsorption
Remark: Intestinal absorption of labelled fatty acids (including decanoic acid) was investigated in the rat. The common bileand pancreatic duct was diverted, and a loop of the duodenumcannulated 24 hours later. The lipid mixture was introducedinto each experimental loop, and the loop was then removed within the next 15 minutes.

Radioactivity distribution studies confirmed that these fatty acids are absorbed in their non-esterified form, and that they are absorbed much more rapidly than oleic acid. autoradiographic studies showed that the medium chain fatty acids are taken uo in a molecular or aggrgate form, leave the epithelial cells by way of the lateral plasma membrane, and are then found in the blood capillaries.

Source: Unichema Chemie GmbH Emmerich
Test substance: 3H-labelled decanoic acid

(74)

Type: Biochemical or cellular interactions
Remark: The vasodilatory effects of various naturally occuring fattyacids (including decanoic acid) was investigated using humanbasilar and umbilical arteries. Test concentrations ranged from 4uM to 4mM.

Decanoic acid was the most potent arterial relaxant. This was especially evident at 40 and 400uM. The basilar artery was more responsive to decanoic acid than the umbilical artery (EC50 63 and 780uM respectively). The relaxation wasindependent of endothelium, and was not related to the weak capacity of decanoic acid to inhibit Ca2+-induced contractions of K+-depolarised basilar arteries. Decanoic acid also inhibited contractions elicited by KCl, serotonin and the thromboxane analogue U46619.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(75)

Type: Biochemical or cellular interactions
Remark: Traditionally, critically ill patients requiring hospital nutrition support were infused with an all-glucose TPN (total parenteral nutrition) system. This has a number of drawbacks, and there is a need for a better lipid system to satisfy the fuel requirements of these patients.

The clinical situations requiring TPN are associated with metabolic processes mediated by insulin. Therefore the authors used an isolated perfused mouse islet model in this study. Various medium chain fatty acids (including decanoicacid) were tested for their ability to stimulate insulin secretion.

Decanoic acid was a potent stimulator in this model.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(76)

Type: Cytotoxicity
Remark: A prokaryote (the cell wall-less microbe Acholeplasma laidlawii) and an eukaryote (the human B-cell line F4) were exposed to decanoic acid and it's perfluorinated counterpart(nonadecafluoro-n-decanoic acid - NDFDA). Both materials caused cytolysis and cytotoxicity to both cell types, depending on the concentrations used.

At 0.5mM NDFDA or decanoic acid no effects were observed, but higher concentrations were lethal. It appeared that a membrane target was involved.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(77)

Type: Cytotoxicity
Remark: The antimicrobial activities of 7 saturated fatty acids (including decanoic acid), their monoglycerides and sucrose esters was investigated.

Decanoic acid had strong fungicidal activity towards Aspergillus niger, Penicillium citrinum, Candida utilis and Saccharomyces cerevisiae.

Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(78)

Type: Metabolism
Remark: 5 human patients were given an oral dose of 14C-labelled decanoic acid in olive oil. 51.8% of the 14C label had beenrecovered 2.5-4 hours of administration.

Source: Unichema Chemie GmbH Emmerich

(55)

Type: other
Remark: A good summary of biological data for decanoic acid is givenin this monograph.
Decanoic acid was given GRAS (generally regarded as safe) status by FEMA (1965), is approved by the FDA for food use (21 CFR 121.1070) and was included by the Council of Europe (1974) at a level of 10ppm in the list of artificial flavouring substances that may be added to foodstuffs without hazard to public health.

Source: Unichema Chemie GmbH Emmerich

(79)

Type: other
Remark: Estimating infant exposure from breast milk depends on 6 substance-related and one maternal factors:

- ionisation constant (pKa)
- protein binding
- molecular weight
- chemical/physical interaction
- elimination/metabolism
- lipid solubility
- maternal blood flow.

Decanoic acid is very lipid soluble; a log octanol/water partition coefficient of 4.09 is reported. This indicates that decanoic acid has the potential to transfer to breast milk. However, no data are presented for the other factors,so no conclusions can be drawn for decanoic acid.
Source: Unichema Chemie GmbH Emmerich
Test substance: Decanoic acid

(80)

Type: other
Remark: The insecticidal properties of a mixture of fatty acids was examined in two Drosophila species (D. mojavensis and D. nigrospiracula), using two cacti (agria and organpipe) as food source.

Triplicate groups of 50 larvae were exposed to each food source, and given 30 days to emerge into adults.

Decanoic acid (0.5% and 1.0%) was lethal to all D. nigrospiracula larvae. D. mojavensis was more tolerant, with viabilities of 76% and 9.3% at 0.5% and 1.0% decanoic acid respectively. Viability was 83-86% in the controls.
Source: Unichema Chemie GmbH Emmerich
Test substance: Various fatty acids (C6-C14) occur naturally in the two cacti used in this study (34.0% in agria and 39.3% in organpipe). These fatty acids were added to a saguaro rot base at 0.5% and 1.0% on a dry weight basis.

(81)

Type: other
Remark: Six lactating cows were used to determine the effect of a medium-chain fatty acid (MCFA) supplement on the fatty acid composition of milk. The diets were supplemented with 300mlMCFA for days 1-10, and 500ml MCFA for days 11-21.

Milk yield and milk protein content were not affected, but milk fat concentration was increased. Minor changes were observed in milk fatty acid composition, but these were unexplained.
Source: Unichema Chemie GmbH Emmerich
Test substance: Up to 500ml of even-carbon medium chain triglyceride (containing 35% decanoic acid).

(82)

Type: other

Remark: Decanoic acid occurs naturally in various edible and cosmetic oils, e.g. coconut oil (up to 9.7%), bay tree oil (37%), and butter fat (2.7%).

Decanoic acid is used in the manufacture of esters for artificial fruit flavours and perfumes.

Source: Unichema Chemie GmbH Emmerich

(83) (84)

Type: other

Remark: The permeability of the blood-brain barrier to 15 14C-labelled organic acids was studied by injecting the testacids into the common carotid artery of rats, and decapitating the rat 15 seconds later.

Uptake of straight-chain saturated acids increased with chain length, and was virtually complete at C6. No measurable uptake of di- or tr-carboxylic acids was observed. The uptake of decanoic acid was 88%.

Source: Unichema Chemie GmbH Emmerich

Test substance: Decanoic acid

(85)

5.11 Experience with Human Exposure

Remark: Children who suffer frm seizures which are not controlable by drugs have apparently been successfully treated with MCT (medium chain triglyceride) diet. The MCT diet is an emulstion containing primarily (81%) octanoic acid, but alsocontains 15% decanoic acid.

In this study 15 children were receiving 50-60% of their energy requirements from the MCT emulsion. Blood samples were analysed for decanoic and octanoic acid levels. There was a wide variation in absolute levels, possibly due to poor patient compliance, but all patients showed low levels in the mornings, rising to high levels in the evenings. This suggested that both acids are rapidly metabolised.

This study did not demonstrate a relationship between MCT diet and siezure control.

Source: Unichema Chemie GmbH Emmerich

Test substance: Decanoic acid

(86)

Remark: A medium chain triglyceride (1g/kg; containing 17% decanoic acid) was given to 10 men and 4 women. They received 2 separate doses, one week apart.

Total plasma cholesterol was lowered after 35 weeks on a triglyceride diet (males only; females had normal cholesterol levels). The triglyceride diet contained 25% decanoic acid.

Source: Unichema Chemie GmbH Emmerich

(87)

Remark: Quantative evaluation of medium and long chain fatty acids in blood samples from healthy children and 7 children suffering from Reye's syndrome showed a significant increasein C8-C10 fatty acids in three of the children with Reye's syndrome.

The authors hypothesised that the fatty acids were the causeof a number of adverse effects, leading to hypoglycaemia andhyperammonaemia.

Source: Unichema Chemie GmbH Emmerich

(45)

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7.1 Risk Assessment

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REFERENCE 3

HERA

Human & Environmental Risk Assessment

on ingredients of

European household cleaning products

Fatty Acid Salts

Human Health Risk Assessment

Draft for Public Comment

June, 2002

Contents

2. Executive Summary

Fatty acid salts (soap) are a widely used class of anionic surfactants. They are used in household cleaning products, cosmetics, lubricants (and other miscellaneous industrial applications) and coatings. Uses in household cleaning products, the scope of this HERA assessment, include fabric washing products, fabric conditioners, laundry additives, and surface and toilet cleaners.

According to data received from a survey conducted among detergent formulator companies, an overall annual tonnage of 71306 tonnes of fatty acid salts for use in HERA applications was estimated. This was compiled using data from 4 out of the 6 main formulator companies.

Fatty acid salts are of low acute toxicity. Their skin and eye irritation potential is chain length dependent and decreases with increasing chain length. They are not skin sensitisers. The available repeated dose toxicity data demonstrate the low toxicity of the fatty acids and their salts. Also, they are not considered to be mutagenic, genotoxic or carcinogenic, and are not reproductive or developmental toxicants.

Accidental ingestion of fatty acid salt containing detergent products is not expected to result in any significant adverse health effect. This assessment is based on toxicological data demonstrating the low acute oral toxicity of fatty acid salts and the fact that not a single fatality has been reported in the UK, following accidental ingestion of detergents containing fatty acid salts.

The estimated total human exposure to fatty acid salts, from the different exposure scenarios for the handling and use of detergent products containing fatty acid salts, showed a margin of exposure (MOE) of 258,620. This extremely large MOE is large enough to be reassuring with regard to the relatively small variability of the hazard data on which it is based. Also, in the UK, the recommended dietary fatty acid intake by the Department of Health is about 100 g of fatty acids per day or 1.7 g (1700 mg) of fatty acids per kilogram body weight per day. This exposure is several orders of magnitude above that resulting from exposure to fatty acid salts in household cleaning products. .

Based on the available data, the use of fatty acid salts in household detergent and cleaning products does not raise any safety concerns with regard to consumer use.

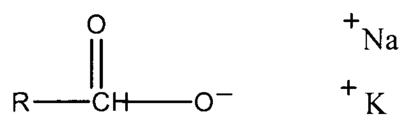
3. Substance Characterisation

Fatty acid salts are a widely used class of anionic surfactants. The applications which are covered by the scope of HERA include use in fabric washing products, fabric conditioners, laundry additives, and surface and toilet cleaners. In addition, there are a number of uses which are not covered by HERA. These include cosmetics, lubricants (and other miscellaneous industrial applications) and use in coatings.

3.1. CAS No and Grouping information

The category for this assessment is defined as the salts of monocarboxylic acids bearing a straight, even numbered fatty acid chain, ranging in number of carbon atoms from 10 to 22. The C16 to C22 members of the group may be saturated or unsaturated (unsatd) with a carbon-carbon double bond.

The fatty acids salts grouping consists of both discrete chemicals with an incremental and constant change across its members (carbon chain length) and commercial mixtures that are composed of fatty acids salts with a range of carbon chain lengths. The chemical structure of the category is:



where R contains from 9 to 21 carbon atoms and the higher fatty acid chain lengths may be saturated or unsaturated, with potassium or sodium salts included.

3.2. Chemical structure and composition

Table 1 covers the CAS numbers provided by 4 out 6 formulator companies. Although clearly important from a Regulatory perspective, the environmental assessment is not based on CAS Nos., but on the product composition and specifically carbon chain length distribution - which is key to the environmental profile of this family. Whilst fatty acids are used in the initial starting list of materials, the final formulation of products covered through this assessment can be expected to contain only fatty acid salts. Thus, the salts of fatty acids only are considered here. Data for fatty acids have been used only for (comparative) read across purposes in the absence of data for the salts.

Table 1 – Chemicals, CAS Numbers, Synonyms, and Structural Composition

CAS No.	Compound	Synonyms	Chain length
Fatty Acid Salts			
629-25-4	Dodecanoic acid, sodium salt	Sodium laurate	12
143-18-0	9-Octadecenoic acid, potassium salt	Oleic acid, potassium salt; Potassium oleate	18
143-19-1	9-Octadecanoic acid, sodium salt	Oleic acid, sodium salt; Sodium oleate	18
822-16-2	Octadecanoic acid, sodium salt	Stearic acid, sodium salt; Sodium stearate	18
2272-11-9	9-Octadecanoic acid (Z)-, compd with 2-aminoethanol (1:1)	Monoethanolamine oleate	20
85408-69-1	Fatty acids, C8-C18 and C16-18 unsatd. Sodium salts	-	16-18
Fatty Acids			
143-07-7	Dodecanoic acid	Lauric acid	12
90990-09-3	Fatty acids, C10-14	-	10-14
67701-01-3	Fatty acids, C12-18	-	12-18
67701-03-5	Fatty acids, C16-18	-	16-18
67701-06-8	Fatty acids, C14-18 and C16-18 unsatd	-	14-18
85711-54-2	Fatty acids, rape oil	-	18-22
68424-37-3	Fatty acids C14-C22	-	14-22

Due to the lim ited availability of m easured p hysical-chemical data f or the f atty acid sa lts, these data have been generated m ostly using predicted values from the EPI WIN program (see Appendix I).

The available data dem onstrate that the m elting point increases with in creasing chain length. Unsaturation results in decreased melting points in comparison to the saturated analogue. The salts of the fatty acids g enerally have higher melting points compared to their co rresponding fatty acid.

The relevance of the boiling point endpoint for the salts of the fatty acids is questionable, as these chem icals are ex pected to d ecompose prior to reaching boiling tem peratures. For saturated linear fatty acids, the boiling point increases with increasing carbon chain length.

The vapour pressure of the salts of single or m ixed fatty acids are expected to be low. Due to lack of m easured data f or the fatty acid s alts predicted values based on estim ated log Kow have been generated by EPI WIN. Available data for members of the fatty acids themselves indicate that these chem icals have very low vapour pressures. Am ong the fatty acids, vapour pressure decreases with increasing chain length.

For fatty acids the partition co-efficient increases with increasing chain length.

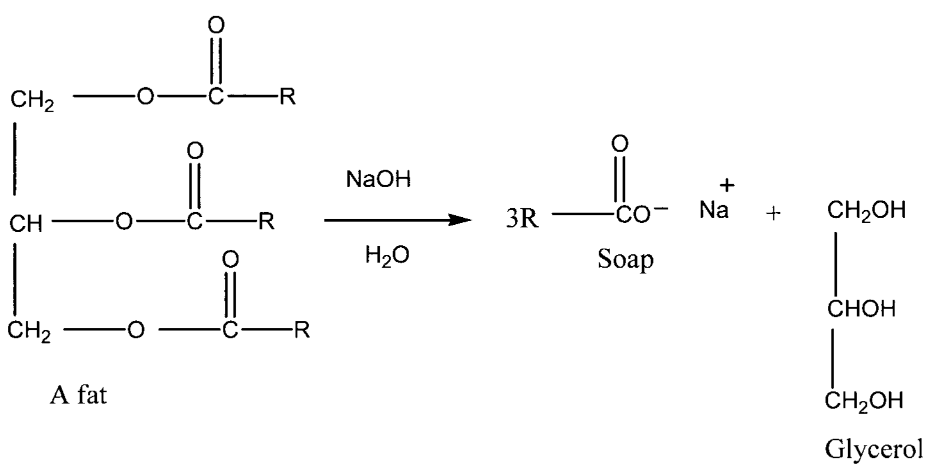
Available data for the s alts of the f atty acids indicate that the salts, not unexpectedly, have much greater water so lubility than the free aci ds, which demonstrate that water solubility decreases with increasing chain length.

Physical-Chemical data are provided in Appendix I.

3.3 Manufacturing Route and Production/Volume Statistics

According to data received from AISE the estimated annual tonnage of fatty acids salts produced for use in household cleaning products in Europe is 71306 tons. This has been compiled from 4 out of the 6 main formulator companies.

Soaps are produced by the saponification of fat with alkali. The production process was invented by Leblanc in 1791, when he found a process for producing soda (Na_2CO_3) and thus NaOH became commercially available for the saponification of fatty acids (Moreno *et al.* 1993; Bruschweiler *et al.* 1988). The saponification of fats is given in figure 1.



Where R = C9 – C21 aliphatic chains

Figure 1: Saponification of fats (from BKH, 1994)

The crude soap curds contain glycerol and excess alkali but purification can be effected by boiling with a large amount of water, followed by precipitation of the pure sodium carboxylate salts on addition of sodium chloride (McMurry, 1984 *cited in* BKH, 1994).

3.4. Use applications summary

Tonnage used in HERA applications (HERA Tonnage)

To determine the total fatty acid salt tonnage used in products falling within the scope of HERA (i.e., household detergents and cleaning products), a survey was conducted among detergent formulator companies (data from members of AISE). The data received from the 4 of the 6 major fatty acid salt formulators provided an overall estimated annual tonnage of 71306 tonnes for HERA applications. In addition, the data provided an estimated distribution between carbon chain lengths. This chain length distribution is not derived for a 100% of the total tonnage but for one which is greater than 80% of the total. The distribution is shown in Table 2.

Table 2. Tonnage of fatty acid salts within the scope of HERA, determined via AISE survey

	Estimated Carbon Distribution of Fatty acid salts (% weight)	Tonnage of fatty acid salts (tonnes/annum (tpa))*
C10	1.1	784
C12	37.2	26526
C14	11.8	8414
C16	17.3	12336
C18	31.8	22675
>C18 **	0.8	570
Total		71306

* These values are calculated from % chain distribution and total tonnage of 71306 tonnes per annum.

** This equates to predominantly C22

5. Human Health Assessment

5.1 Consumer Exposure

5.1.1 Product types

Data supplied by the formulating companies shows that fatty acid salts (soap) are used in fabric washing powders, tablets and liquids/gels, in fabric conditioners, laundry additives and in surface and toilet cleaner liquids. The salts of the fatty acids considered in this assessment are the sodium and potassium salts only. The level of soap found in fabric washing products ranges from approximately 0.1-10.5% in regular powder, 2-20% in regular liquid, 0.1-3.4% in compact powder, 4-10% in compact liquid, 0.7-2% in tablets and 13.1-15.1% in compact gels. The maximum level found in fabric conditioners is 0.75%, while levels of 0.1-3.0% can be found in surface cleaners (with the gel containing potentially the highest levels) and 0.55-1.9% in toilet cleaners. Table 1 in Section 3.2 (and Table 1 in Appendix II) gives the chemical names, synonyms and carbon chain lengths of the chemicals considered in this assessment.

5.1.2 Consumer Contact Scenarios

Fabric washing powders and liquids as well as fabric conditioners are used in two ways, either in the washing machine or in a bowl for hand washing. Surface and toilet cleaner liquids are applied directly onto the surface or into the toilet bowl. Hence, the potential for consumer contact is identified as follows:

- Dermal contact:-
  - Contact with the washing solution
  - Contact with concentrated paste of product used in fabric pre-treatment
  - Contact with clothes containing deposited product
- Contact via inhalation:-
  - Pouring the product from the container into the machine/bowl (does not apply to liquid, tablets or gel)
  - Inhalation of aerosols generated by spray cleaners
- Oral ingestion:-
  - Direct accidental or intentional ingestion of product
  - Indirect exposure via the environment
- Other Exposures – eye exposure:-

- Splashing of products into eye

5.1.3 Consumer contact estimates

There is a consolidated overview concerning the habits and uses of detergents and surface cleaners in Western Europe, which was tabulated and issued by the European Soap and Detergent Industry Association, AISE (AISE, 2002). This list reflects the consumer's use of detergents in g/cup, tasks/week, duration of task and other uses of products and is relevant in providing data reflecting consumer exposure. It can be used in calculating the following:

5.1.3.1 Dermal contact

Consumers may be exposed to fatty acid salts via skin contact with washing solutions, which contain fatty acid salts. Relevant exposure scenarios are direct contact with the product, hand washing of clothes, contact with the concentrated paste of products used in fabric pre-treatment and contact with clothes containing deposited product.

Direct Skin Contact: Hand-washed Laundry

The concentration of laundry detergent in hand washing solutions is approximately 1% (10 g/l) (AISE, 2002). The highest concentration of fatty acid salts in laundry detergents is 20% (for liquid detergent). For this reason in a worst case assumption, the hands and forearms of the consumer could be exposed to an estimated fatty acid salts concentration of up to 2.0 g/l (= mg/ml). The estimated surface of the hands and forearms, exposed to the washing solution is 1980 cm^2 (EU Technical Guidance Document (EU TGD), Part I, Annex VI).

Soap is a surface active agent and soap anions will form a film on the surface. Therefore, the concentration on the surface will be different from the body of the suspension. However, assuming a film thickness of 100 µm (0.1 mm or 0.01 cm) (EU TGD, Part I, Annex VI) on the hands and a percutaneous absorption of 1% (0.01) for ionic substances (Schaefer and Redelmeier, 1996) (the ionised acid form of the fatty acids is less easily absorbed than the non-ionised form, therefore the 1% (0.01) used here is a worst case assumption) in a 24 hour exposure period, the following amount of fatty acid salts absorbed via skin can be calculated:

Surface area of hands and forearms x film thickness x fraction absorbed x fatty acid salt concentration = amount absorbed

$$1980 \text{ cm}^2 \times 0.01 \text{ cm} \times 0.01 \times 2.0 \text{ mg/ml } (\text{cm}^3) = 0.40 \text{ mg}$$

0.40 mg fatty acid salts absorbed in 24 hours

Assuming 10 minutes contact time per task and a very conservative maximum task frequency of 21 washes per week (3 per day) (AISE, 2002), the total daily contact time is 30 minutes. Therefore, a correction factor of [(0.40 mg/day) x (1/24 day/hr) x (30/60hr)] is used yielding an assumed absorption of **8.3 x 10^{-3} mg.**

Based on a body weight of 60 kg the estimated systemic dose of fatty acid salts would be equal to:

$Exp_{sys\ (direct\ skin\ contact)}$ = 1.4 x 10^{-4} mg/kg body weight per day

Direct skin contact: Contact with laundry tablets/powder/liquid

Contact with laundry tablets may occur during unwrapping the tablets and placing them into the washing machine. However, the contact time is very low (<1 min) and only the tips of thumb and index finger of one hand are exposed so the amount absorbed percutaneously is considered insignificant. Some parts of the body, mainly the hand, might also come into contact with washing powder/liquid when transferring the product from the container into the machine. Contact time during these scenarios is very low and can be assumed to be a few seconds, the skin area affected is small and exposure occurs only occasionally and not regularly with product use. Hence, the systemic fatty acid salts exposure resulting from this scenario is also considered to be negligible.

Direct skin contact: Contact via pre-treatment of clothes

Commonly, clothing stains are spot-treated by hand with detergent. If a powdered detergent is used, a paste of about 60% [600 mg/ml powder] (AISE, 2002) will be used or a liquid will be applied directly. The highest concentration of fatty acid salts in laundry powder (laundry regular) is 10.5%. Therefore, the highest concentration of fatty acid salts in hand washing paste will be 63 mg/ml. The highest concentration of fatty acid salts in liquid laundry detergents amounts to 20% (200 mg/ml). Because liquid detergents may be used for pre-treatment, the worst case value of 200 mg/ml will be used in the calculation. The skin surface area exposed will be the hands only (840 cm^2) (EU TGD, Part I, Annex VI).

Again assuming a film thickness of 100 µm on the hands and a percutaneous absorption of 1% for ionic substances in 24 hour exposure time, the following amount of fatty acid salts absorbed via skin can be calculated:

Surface area of hands x film thickness x fraction absorbed x fatty acid salt concentration = amount absorbed

$$840\ cm^2 \times 0.01\ cm \times 0.01 \times 200\ mg/ml\ (cm^3) = 16.8\ mg$$

16.8 mg fatty acid salts absorbed in 24 hours

Under the very conservative assumptions of 10 min highest contact time per task and a maximum task frequency of 1 wash pre-treatment per day, the total daily contact time adds to 10 minutes. Assuming such very conservative daily duration of exposure the amount of absorbed fatty acid salts per day can be calculated as [(16.8 mg/day) x (10/60 hr) x (1/24 day/hr)] = **0.12 mg.**

Based on a body weight of 60 kg the estimated systemic dose of fatty acid salts would be equal to:

$Exp_{sys\ (direct\ skin\ contact)}$ = 2.0 x 10^{-3} mg/kg body weight per day

This exposure estimate can be regarded as very conservative. Typically, consumers pre-wet the laundry before applying the detergent for pre-treatment or conduct pre-treatment under running tap water. Both practices lead to a significant dilution which is not reflected in this exposure estimate. It should also be considered that only a fraction of the two hands' surface will actually be exposed. The assumption that both hands will be fully immersed leads to a likely overestimate of the true exposure.

Indirect skin contact: Transfer of FAS from clothing

Residues of components of laundry detergents may remain on textiles after washing and can transfer from the textile to the skin. Rodrgiuez *et al.* (1994) determined that the amount of fatty acids deposited on fabric after 10 repeats of a typical washing process with a typical laundry detergent was in the order of 13.4 g of fatty acids per kg of fabric.

The indirect dermal exposure resulting from the transfer of fatty acid salts from clothing can be calculated using the equation as described in Appendix D of the HERA guidance document:-

$$\boxed{\mathbf{EXP_{sys} = F_1 \times C' \times S_{der} \times n \times F_2 \times F_3 \times F_4 / BW}}$$

Where F_1 percentage (%) weight fraction of substance in product: **20%** (0.2)

C' product load in [mg/cm^2]: **1.34×10^{-1} mg/cm^2***

S_{der} surface area of exposed skin [cm^2]: **17,600 cm^2 (excludes heads and hands)**

n product use frequency [events/day]: 1 (not used)

F_2 percentage (%) weight fraction transferred from medium to skin: **1%** (Vermeire *et al.* 1993)

F_3 percentage (%) weight fraction remaining on skin: **100%** (worst case assumption)

F_4 percentage (%) weight fraction absorbed via skin: **1%** (Schaefer and Redelmeier, 1996)

BW body weight in kg: **60 kg**

* C' was determined by multiplying the experimental value of the amount of fatty acids deposited on fabric after a typical wash (i.e. 13.4 g/kg) (Rodriguez *et al.* 1994) times an estimated value of the fabric density (FD = 10 mg/cm^2) (P&G unpublished internal data, 1996)

$$\mathbf{EXP_{sys} = F_1 \times C' \times S_{der} \times n \times F_2 \times F_3 \times F_4 / BW}$$

$$\mathbf{EXP_{sys}} = 0.2 \times (1.34 \times 10^{-1}) \times 17{,}600 \times 0.01 \times 1 \times 0.01 / 60$$

$$\boxed{EXP_{sys\ (indirect\ skin\ contact)} = 7.9 \times 10^{-4} \text{ mg/kg body weight/day}}$$

5.1.3.2 Oral exposure

There is no significant source of oral contact from the recommended use of soaps in detergent products.

Accidental Ingestion

The accidental or intentional overexposure to fatty acid salts directly is not considered to be a likely occurrence for consumers, but it may occur via household detergent products containing fatty acid salts. In the UK, the Department of Trade and Industry (DTI) produce an annual report of the home accident surveillance system (HASS). The data in this report summarises the information recorded at accident and emergency (A & E) units at a sample of hospitals across the UK. It also includes death statistics produced by the Office for National Statistics for England and Wales. The figures for 1998 show that for the representative sample of hospitals surveyed, there were 33 reported accidents involving detergent washing powder (the national estimate being 644) with none of these resulting in fatalities (DTI, 1998). In 1996 and 1997, despite their being 43 and 50 reported cases, respectively, no fatalities were reported either.

Also, considering the high levels of fatty acids that are present in the diet, it is extremely unlikely that accidental ingestion of a household cleaning product would result in over exposure to fatty acids or their salts, and any adverse effects seen are unlikely to be due to these chemicals.

Indirect Exposure

There are no data available on the levels of soap present in drinking water. However, in an environmental hazard assessment of soaps by BKH (1994), it is reported that "due to strong adsorption and poor water solubility of calcium salts, soaps are almost completely removed from raw sewage by normal sewage treatment plants". Any soap remaining will be further removed by drinking water treatment processes so the amount of soap present in drinking water is likely to be insignificant.

Indirect Exposure via the diet

By far the most significant exposure to fatty acids and their salts is via the diet as fatty acids are present in large quantities in the diet. In the UK, the Department of Health have set dietary reference values for fat and recommend that total fatty acid intake should average 30 per cent of total dietary energy including alcohol (DoH, 1991). This equates to about 100 g of fatty acids per day or **1.7 g of fatty acids per kg body weight (1700 mg/kg body weight per day)**.

5.1.3.3 Inhalation Exposure

Inhalation exposure from pouring the product from the container into the machine/bowl

Fabric washing powders are manufactured to rigorous specifications of particle size, enhanced by the exclusion of particles small enough to be inhaled into the lungs. Tests on fabric washing powders over many years have shown a very low level of dust in these products, and within the dust, the level of respirable particles is extremely low. It has been estimated that a cup of fabric washing powder (200 g) can generate 0.27 µg of dust (Van de Plassche *et al.*

1998), giving rise to a m aximum e xposure by inhalation of **0.028 µg of fatty acid salts** (assuming 10.5% of material in product).

Hence, intake via inhalation = $0.028 \times 10^{-3}/60 \times 3^{*}$ = **1.4×10^{-6} mg/kg body weight/day**

*Assuming 21 washes per week (21/7 = 3) (AISE, 2002)

Lint formation during drying of fabrics in tum ble-driers which vent indoors is not considered to contribute to inhalation exposure to fatty acid salts, since washed fabrics do not contain any significant amount of fatty acid salts (see above).

Inhalation of aerosols generated by spray cleaners

Fatty acid s alts are also present in surface cl eaning sprays at a m aximum concentration of 0.1%. The HERA guidance document specifies th e algorithm to be used for calculation of consumers' worst-case exposure to aerosols generated by the spray cleaner:

$$\mathbf{Exp_{sys} = F_1 \times C` \times Q_{inh} \times t \times n \times F_7 \times F_8 / BW}$$

F_1 percentage weight fraction of substance in product **0.1%** (worst case)

C` product concentration in air: **0.35 mg/m^3** * (P&G unpublished data)

Q_{inh} ventilation rate **-0.8 m^3/h** (EU TGD)

t duration of exposure - **10 min** (0.17h) (AISE, 2002)

n product use frequency (tasks per day) - **1** (AISE, 2002)

F_7 weight fraction of respirable particles - **100%**

F_8 weight fraction absorbed or bioavailable - **75%** (EU TGD)

BW body weight **60 kg** (EU TGD)

* this value was obtained by experimental measurements of t he concentration of aerosol particles smaller than 6.4 microns in size which are generated upon spraying with typical surface cleaning spray products [Note is the value of 6.4 microns acceptable; sometimes a cut-off value of 10 micron is used.

$$\mathbf{Exp_{sys} = F_1 \times C` \times Q_{inh} \times t \times n \times F_7 \times F_8 / BW}$$

$Exp_{sys\ (inhalation\ of\ aerosols)}$ = [(0.001) x (0.35 mg/m^3) x (0.8 m^3/hr) x (0.17 hr) x (0.75)] / 60 kg **$Exp_{sys\ (inhalation\ of\ aerosols)}$ = 6.0×10^{-7} mg /kg body weight per day**

5.1.3.4 Other exposures (eye exposure)

Accidental exposure of the eyes to fatty acid salts will occur in consumers only via splashes or spills with a formulated product. Therefore, the eye irritation potential has to be considered in the context of accidental exposure.

Table 3 - Total Consumer Exposure (All Routes) from household cleaning products

Route	Exposure to soap (mg/kg/day)
1. Dermal	
Hand laundry	1.4×10^{-4}
Fabric pre-treatment	2.0×10^{-3}
Wearing laundered fabric	7.9×10^{-4}
TOTAL DERMAL	***2.9×10^{-3}***
2. Oral	
Accidental Ingestion	--
Indirect Exposure via Drinking Water	Negligible
TOTAL ORAL	***Negligible***
3. Inhalation	
Pouring product	1.4×10^{-6}
Spray cleaner	6.0×10^{-7}
TOTAL INHALATION	***2.0×10^{-6}***
TOTAL (ALL ROUTES)	**2.9×10^{-3}**

5.2 Hazard Assessment

5.2.1 Summary of available toxicological data

Introduction

The acid and alkali salt forms of the same chemical are expected to have many similar physicochemical and toxicological properties when they become bioavailable; therefore, data read across is used for those instances where data are available for the acid form but not the salt, and vice versa. This position is based on experimental studies that have clearly demonstrated a high degree of similarity between the toxicokinetics and toxicodynamics of acid and salt forms of the same chemical (BASF, 2001).

A general premise in regulatory toxicology is that testing an acid form of a chemical is representative of the testing that chemical as an alkali salt. In the gastrointestinal tract, acids and bases are absorbed in the undissociated (non-ionised) form by simple diffusion or by facilitated diffusion. In general, the amount of dissociation of acids and bases is determined by the pKa values of the substance and the pH of the environment. The pH of the stomach varies between 1-3 and in the intestines, pH values between 5 and 8 are reported. In an acidic environment, acids will be present mainly in the non-ionised form. The amount of dissociation depends on the strength of the acid. Strong acids may be dissociated to some extent in very acidic environments like the stomach, but weaker acids will occur mainly undissociated (BASF, 2001).

It is expected that both the acids and the salts will be present in (or converted to) the acid form in the stomach. This means that for both types of parent chemical (acid or salt) the same compounds eventually enter the small intestine, where equilibrium, as a result of increased pH, will shift towards dissociation (ionised form). Hence, the situation will be similar for compounds originating from acids and therefore no differences in uptake are anticipated (BASF, 2001).

5.2.1.1 Acute Toxicity

As all the data below have been taken from secondary published sources and not from the original studies, the data have been rated as class 4 (i.e. not assignable) using the method described by Klimisch *et al.* (1997), unless otherwise stated.

Acute oral toxicity

Given the assumption that the salts of fatty acids will exhibit a similar toxicity profile as the comparable free acids, the available data on the fatty acids in Table 4 can be used to estimate the toxicity for the salts for which data are lacking. For example, both stearic acid and sodium stearate (C18) have reported LD50 values of >5,000 mg/kg body weight.

The available data for fatty acids provide a clear picture of low acute toxicity for this class of chemicals. All oral LD50 values were greater than 2,000 mg/kg, with little mortality being observed even at the highest doses tested in the studies (IUCLID, 2000c, 2000e, 2000f, 2000g; Clayton & Clayton, 1982; CIR, 1987).

The available data for the fatty acid salts also indicate that these are of low acute toxicity. For example, an acute oral LD50 value of >5,000 mg/kg (highest dose tested) has been reported for sodium soap. This test was done according to GLP and OECD Guideline 401 (IUCLID, 2000f), while in another study also done to GLP and according to Directive 84/449/EEC, B.1, an LD50 value of >2,000 mg/kg (highest dose tested) was reported for fatty acids, C16-18 and C18-unstad., sodium salts (IUCLID, 2000f).

Any toxic effects, such as excessive salivation, diarrhoea, central nervous system depression, loss of reflex actions or coma, shown at higher doses, decrease in severity with an increase in the chain length of the fatty acid (Pi-Sunyer *et al.,* 1969). These reported effects are a result of the high doses administered and the fact that unlike humans rats don't have a vomiting reflex. Therefore, these high dose effects are not considered relevant for human exposure.

Summary: The available data indicate that the fatty acid salts exhibit a very low order of toxicity following acute exposure via the oral route.

Acute Inhalation Toxicity

The physical/chemical properties of fatty acid salts and their normal usage scenarios dictate that the primary route of exposure will be dermal which is consistent with the available data, with very limited data on the effects of acute inhalation of fatty acids or their salts located. In a study in which rats were exposed for 8 hours to saturated vapours of mixed isomers of decanoic acid (C10) no deaths were observed (IUCLID, 2000c).

Summary: The very limited data do not indicate that adverse effects would be expected following inhalation of fatty acid salts. In addition, this is not expected to be a significant route of exposure to these chemicals.

Acute Dermal Toxicity

As with the acute oral data, the available acute dermal toxicity data for the fatty acids (and their salts) provide a clear picture of low acute toxicity for this group of chemicals. All dermal LD50 values were greater than >2,000 mg/kg (BIBRA, 1996; IUCLID, 2000e; Clayton & Clayton, 1982; CIR, 1982, 1987).

In a dermal study in which concentrations of sodium stearate (C18) ranged between 10-25% in a 20% bath soap detergent form, the LD50 was >3000 mg/kg (highest dose tested) (CIR, 1982). In a dermal study in guinea pigs, application of commercial grade oleic acid (3,000 mg/kg) produced no deaths and no signs of toxicity. The number of applications was not stated (CIR, 1987).

Summary: The available data indicate that fatty acids (and their salts) are of low acute toxicity by the dermal route.

Table 4 – Acute toxicity of fatty acids and their salts

Test Material	CAS No.	Chain Length	Species /route	LD50 (mg/kg bw)	Reference
Decanoic acid (capric acid)	334-48-5	10	Rat/oral Rat/dermal Rat/inhal.	3,320 >5,000 No deaths with 8hr conc. vapour	IUCLID, 2000c BIBRA, 1996 BIBRA, 1996
Dodecanoic acid (lauric acid)	143-07-7	12	Rat/oral	12,000	Clayton & Clayton, 1982
Hexadecanoic acid (palmitic acid)	57-10-3	16	Rat/oral Rabbit/dermal	>10,000 >2,000	CIR, 1987 CIR, 1987
Octadecanoic acid (stearic acid)	57-11-4	18	Rat/oral Rabbit/dermal	>5,000 >5,000	Clayton & Clayton, 1982

Octadecanoic acid, Na salt (sodium stearate)	822-16-2	18	Rat/oral Rabbit/dermal Rabbit/dermal	>5,000 >10 ml/kg (formulation) >3,000	CIR, 1982 CIR, 1982 CIR, 1982
9-Octadecenoic acid (oleic acid)	112-80-1	18	Rat/oral Guinea pig/dermal	>19,243 >3,000	IUCLID, 2000e IUCLID, 2000e
Fatty acids, C14-18 and C16-18 unsat'd.	67701-06-8	16-18	Rat/oral Rat/oral	>5,000 >2,000	IUCLID, 2000f IUCLID, 2000f
Fatty acids, C18-22	90990-11-7	18-22	Rat/oral	>5,000	IUCLID, 2000g

5.2.1.2 Corrosiveness/Irritation

As all the data below have been taken from secondary published sources and not from the original studies, the data have been rated as class 4 (i.e. not assignable) using the method described by Klimisch *et al.* (1997), unless otherwise stated.

Skin Irritation

General

The primary concern with fatty acids is usually of an acute nature arising from the primary irritant effect, particularly of the short chain length acids (carbon chain lengths of C_{16} to C_{18} contribute to a low skin irritation effect). As the molecular weight increases and the water solubility decreases, the irritating capacity in general decreases (Clayton & Clayton, 1982; Madsen *et al.,* 2001).

Human Data

Studies in humans on the relative irritancy of free fatty acids (under occlusive patches) have revealed that the even numbered chain saturated free fatty acids of C_8 through C_{14} chain lengths are the most irritating (Stillman *et al.* 1975). With 0.5 M fatty acids, in most males (total of 10 subjects) there was an erythematous response by the tenth day at the sites of application of C_8 through C_{12}. There was a negligible response to the other fatty acids (C_{14} through C_{18}). By the eighth day of application of the 1.0 M saturated fatty acids, there was an erythematous response in all subjects at the sites of C_8 through C_{12}. There was a negligible response to fatty acids C_{14} through C_{18} (Stillman *et al.* 1975).

Approximately 0.5% aqueous solutions of the sodium salts of decanoic acid (C10) proved irritant to 3-40% of an unstated number of volunteers (no other details available) (BIBRA, 1996), while covered contact (22-24 hr) with 0.25% aqueous sodium decanoate caused weak reactions (presumably of an irritant nature) in two of 25 volunteers. Similar tests with 0.1% apparently elicited no responses (no other details available) (BIBRA, 1996).

Several soap bar formulations with concentrations of myristic acid (C14) of 10, 22.1 and 91.0% were tested for skin irritation using 16 human subjects. A 0.2 ml volume of 8%

aqueous preparations was applied to the ventral skin of the forearm under occlusive patches once daily for 5 days using the Frosch-Kligman soap chamber test. The formulations were considered "slightly" to "moderately irritating", and erythema scores were 1.41, 1.73 and 1.95 on a scale from 0 to 5 for the formulations containing 10, 22.1 and 91% myristic acid, respectively (CIR, 1987).

In a single insult occlusive patch test (SIOPT), commercial grade myristic acid produced no irritation in 17, mild erythema in 2, and moderate erythema in 1 of 20 panellists. The primary irritation index was 0.2 and myristic acid was considered "practically non-irritating" (CIR, 1987).

A single insult, 24 hour, occlusive patch test was conducted on 20 human subjects to determine the skin irritation potential of 0.5% sodium stearate in aqueous solution. The test solution produced no irritation in 16 subjects, and minimal to moderate erythema in four. The investigators concluded that sodium stearate (C18) "exhibited an acceptable and typical soap response" (CIR, 1982).

Animal Data

Tests in animals show that the skin irritation potential of fatty acids decreases with increasing chain length, such that the very short chain acids are corrosive, the medium chain length C10 is irritant, and C12 is minimally irritant. The longer chain lengths, C14 and above, are not irritant (CIR, 1987; Madsen *et al.* 2001). Also, the existence of unsaturated carbon chains and carbon chain lengths of C_{16} to C_{18} contribute to a low skin irritation effect (Madsen *et al.,* 2001).

In a study evaluating the toxicity of nine of the most commonly used commercial grades of fatty acids, both grades of octadecanoic acids (70% stearic acid, 30 % palmitic acid; 45% stearic acid, 55% palmitic acid), myristic acid (C14) and palmitic acid (C16) gave a primary irritation index (PII) of 0. Capric acid (C10) proved to have higher irritancy with a PII of 4.60 (Briggs *et al.* 1976).

A SIOPT of commercial grade lauric acid (C12) (0.5 ml) to intact and abraded sites of the skin of 6 albino rabbits produced slight erythema at both sites after 24 hours which subsided by 72 hours, minimal oedema after 72 hours and a PII of 1.12. Blanching and some coriaceous tissue were noted at a few abraded sites (CIR, 1987).

A 50% solution of a coconut soap (for which lauric acid is the dominant acid) was patch tested in rabbits, guinea pigs and humans. Skin responses were graded at 4, 24 and 48 hours after each patch application. Irritancy judged at 4 hours was negligible in humans, slight in the guinea pig and moderate in the rabbit (Nixon *et al.* 1975).

Sodium soap (composition not stated) was not irritating (concentration used not stated) to rabbits in the acute dermal irritation/corrosion test conducted to GLP and according to OECD Guideline 404 (IUCLID, 2000f).

Pure fatty acid sodium soap was applied to the uncovered skin of rabbits, "hairless" mice and guinea pigs for prolonged periods (five days a week for four and a half weeks – that is 23 applications) in order to represent the exposure of skin during normal working conditions. Following the tests, the skin was removed from the animals and subjected to histological examination. No histological changes were noted and the test material was at the low end of the irritancy scale. However, in patch tests, the fatty acid sodium salt had shown a medium irritancy grade, indicating that, given different conditions of exposure, the same chemical may behave in a different manner in contact with the skin (Brown, 1971). However occlusive patches were used, which is not relevant to the household cleaning product exposure conditions and so is of limited relevance.

In a SIOPT, commercial grade myristic acid (C14) (0.5 ml) was applied to intact and abraded sites on the skin of 6 albino rabbits and the PII was 0. In a "repeat open patch" test using commercial grade myristic acid (0.5 g), all 6 treated albino rabbits developed mild to moderate erythema from 24 to 72 hours. One rabbit developed very slight oedema after the 72-hour scoring (CIR, 1987).

A 100% concentration of sodium stearate (C18) applied as a single dose under occlusive conditions (not relevant to product use conditions) to six albino rabbits caused no irritation (PII = 0.0) (CIR, 1982). In a Draize test, 10-25% sodium stearate in a bath soap and detergent form caused mild irritation in 6 rabbits (PII = 2.2) (CIR, 1982). In a SIOPT of commercial grade stearic acid, transient minimal erythema and no oedema were noted in 9 albino rabbits after a 2-hour exposure period (CIR, 1987).

Summary: Tests in animals and humans show that the skin irritation potential of fatty acids and their salts decreases with increasing chain length, such that the medium chain lengths (C10) are irritant, C12 is minimally irritant and the longer chain lengths, C14 and above, are not irritant.

Eye Irritation

Human Data

Accidental contact of the human eye with soap or soap powder followed by rapid rinsing of the eyes is not expected to cause severe reactions and reactions observed resolve quickly without any permanent damage (Madsen *et al.* 2001).

Animal Data

As with skin irritation, tests in animals also show that the eye irritation potential of fatty acids decreases with increasing chain length, such that chain lengths C10 and C12 are irritant and the longer chain lengths, C14 and above are not irritant (Briggs *et al.* 1976; CIR, 1987).

Instillation of commercial grade lauric acid (C12) into the eyes of 6 albino rabbits produced corneal opacity, mild conjunctivitis, and iritis throughout the 72 hour observation period. An aqueous dilution (8.0%) of a product formulation containing 8.7% lauric acid produced no occular irritation in 6 albino rabbits. A 1% aqueous preparation of a soap formulation containing 1.95% lauric acid was not irritating to treated unrinsed eyes of rabbits (CIR, 1987).

Administration of commercial grade palmitic acid (C16) to the eyes of 6 albino rabbits produced no irritation. Mild to moderate ocular irritation was produced in rabbits by product formulations containing 19.4% palmitic acid (CIR, 1987).

In occular irritation studies, fatty acids (lauric, myristic, palmitic, oleic and stearic acid) alone and at concentrations ranging from 1 to 19.4% in cosmetic product formulations produced no to minimal irritation after single and multiple (daily, 14-day) instillations into the eyes of albino rabbits. Irritation was primarily in the form of very slight conjunctival erythema. A single instillation of lauric acid (as commercially supplied) also produced corneal opacity and iritis (CIR, 1987).

In a study evaluating the toxicity of nine commercial grades of fatty acids, stearic acid (55%-C16, 45%-C18) produced mild conjunctival erythema in two of six rabbits at 24 and 48 hours while all signs of irritation had subsided completely in 72 hours. The other acids fell roughly into the following levels of irritancy; stearic acid (unsaturated) and myristic acid (C14); mild conjunctivitis with complete clearing in 72 hours. Lauric (C12) and capric (C10); corneal opacity and moderate conjunctivitis which did not subside in 72 hours (Briggs *et al.* 1976).

In a Draize eye test, a 100% concentration of sodium stearate (C18) was applied to 6 rabbits and resulted in negligible irritation. On day one, 2/6 conjunctivae appeared necrotic and the irritation scores corresponded to moderate irritation initially, but negligible irritation was recorded by day 4 (CIR, 1982).

Sodium soap was not irritating to rabbits in the acute eye irritation/corrosion test conducted to GLP and according to OECD Guideline 405 (no other details available) (IUCLID, 2000f).

(Z)-Docos-13-enoic acid (C22) was moderately irritating in the rabbit eye in an acute eye irritation/corrosion test conducted to GLP and according to OECD Guideline 405 (no other details available) (IUCLID, 2000e).

Summary: As with skin irritation, tests show that the eye irritation potential of fatty acids and their salts decreases with increasing chain lengths, such that chain lengths C10 and C12 are irritant and the longer chain lengths, C14 and above are not irritant.

5.2.1.3 Sensitisation

As all the data below have been taken from secondary published sources and not from the original studies, the data have been rated as class 4 (i.e. not assignable) using the method described by Klimisch *et al.* (1997), unless otherwise stated.

Human Data

In a skin sensitisation study in 28 volunteers, five 48-hour covered applications of 1% decanoic acid (C10) in petrolatum were made over a 10 day period. The results were negative since none gave positive reactions when challenged 10-14 days after the induction phase with a final 48-hour closed patch test using 1% in petrolatum (IUCLID, 2000a).

No local reactions indicative of sensitisation were seen in 100 subjects patch tested [under unspecified conditions] with a bath soap and detergent formulation containing 0.3-0.75% sodium stearate (BIBRA, 1990).

De Groot *et al.* (1988) reported that 25 subjects showed no sensitisation reactions when exposed to 5% stearic acid (C18) in petrolatum and a 1% aqueous sodium stearate solution.

Animal Data

In two Magnusson and Kligman guinea pig maximisation tests, carried out in conformity with OECD Guideline No. 406 and EC test method B.6 as described in the Annex of EC Directive 84/449/EEC, using two different types of mixed fatty acid sodium salts, no skin sensitisation potential was demonstrated in either material (CIR, 1982).

Sodium soap (composition not stated) did not produce sensitisation reactions (concentration used not stated) in the guinea pig maximisation test which was conducted to GLP and according to OECD Guideline 406 (IUCLID, 2000f).

Summary: Based on the available data, fatty acids and their salts are not expected to have any skin sensitisation potential.

5.2.1.4 Repeated Dose Toxicity

Introduction

In the UK, the Department of Health have set dietary reference values for fatty acids and recommend that total fatty acid intake should average 30 per cent of total dietary energy including alcohol (DoH, 1991). This equates to about 100 g of fatty acids per day or 1.7 g (1700 mg) of fatty acids per kg body weight per day.

The available data demonstrate the low toxicity of fatty acids and their salts, which is consistent with the long history of safe use in foods for both fatty acids and glycerides. Further evidence of their safe use in foods is the fact that a number of regulatory bodies have reviewed data not available to us and concluded that fatty acids and their salts are of low toxicity.

For example, several of the fatty acids are Generally Recognised as Safe (GRAS) by the U.S. Food and Drug Administration (US FDA). Substances that are listed as GRAS include: stearic acid; oleic acid and sodium palmitate. Stearic acid is also included by the Council of Europe (1974), at a level of 4000 ppm, in the list of artificial flavouring substances that may be added to foodstuffs without hazard to public health. In those studies where adverse effects were observed at high doses, these effects were considered to be the result of dietary imbalance in fat intake. With respect to the salts of fatty acids, it is expected that these materials possess similar characteristics as the free acid, for the reasons outlined in 5.2.1.

When decanoic acid (C10) was reviewed by the Joint FAO/WHO Expert Committee on Food Additives, no specific ADI was established, because it was held that the compound's presence in food would not represent a human health hazard. This view was based upon the occurrence of the acid in edible fats and oils with long food-use history as well as data on total daily intakes and the toxicology of the acid (JECFA, 1986). Decanoic was also considered "safe in use" by the EU's Scientific Committee for food in their consideration of Chemically Defined Flavouring Substances (SCF, 1995).

The fatty acids as a group are permitted as direct food additives (21 CFR 172.210, 172.860, 173.340); There are no limitations other than the observance of current good manufacturing practice (21 CFR 174.5) on the use of oleic acid and stearic acids as indirect food additives (21 CFR 175.105, 176.200 and 21 CFR 175.105, 175.300, respectively) (CIR, 1987).

In 1974, the WHO set an unlimited ADI for the salts of myristic (C14), palmitic (C16) and stearic (C18) acids. They stated that myristic, palmitic and stearic acid and their salts are normal products of the metabolism of fats and their metabolic fate is well established. Provided the contribution of the cations does not add excessively to the normal body load there is no need to consider the use of these substances in any different light to that of dietary fatty acids (WHO, 1974; JECFA, 1986).

In Western Europe and North America, the estimated overall consumption of dietary sodium chloride is 5-20 g/day (2-8 g of sodium per day), the average being 10 g/day (4 g of sodium) (WHO, 1996). In the UK dietary reference values (DRV) have been published for potassium. The reference nutrient intake (RNI) for adults is 3.5 g daily (DoH, 1991). Considering the high intake of these individual cations in the diet, exposure to fatty acid salts in household cleaning products will not add excessively to the normal body load.

Oral Toxicity

As all the data below have been taken from secondary published sources and not from the original studies, the data have been rated as class 4 (i.e. not assignable) using the method described by Klimisch *et al.* (1997), unless otherwise stated.

It is worth noting when considering the oral toxicity of fatty acids and their salts, that due to their innocuous nature, fats and oils are commonly used as controls and as vehicles in animal toxicity studies. For example, OECD Guideline 408 (repeated dose 90-day oral toxicity study in rodents) recommends the use of "a solution/ emulsion in oil (e.g. corn oil)" as a vehicle where an aqueous vehicle is not suitable (OECD, 1993).

Fitzhugh *et al.* (1960) fed lauric acid (C12) to five male rats at the 10% level of their diet for 18 weeks. A control group of 5 males was fed concurrently. There were no observable clinical effects, no adverse effects on weight gain, nor was there any mortality. Gross organ pathology and comparison of individual organ weights showed no significant differences between the controls and test animals.

In a 24-week oral study, rats were fed doses of 15% oleic acid (C18) (approximately 7.5 g/kg body weight per day). Normal growth and general good health was reported in the rats and the NOAEL was reported to be >7,500 mg/kg body weight per day (IUCLID, 2000e).

Caprenin, a randomised triglyceride primarily comprising caprylic (C8), capric (C10), and behenic (C22) acids, was administered in a semi-purified diet to weanling Sprague-Dawley rats (25/sex/group) at dose levels of 5.23, 10.23 or 15.00% (w/w) for 91 days. Corn oil was added at 8.96, 5.91 and 3.00%, respectively, to provide essential fatty acids and digestible fat calories. Survival, clinical signs, body weight, feed consumption, feed efficiency, organ weights, organ-to-body-weight ratios, organ-to-brain-weight ratios, haematological values and clinical chemistry parameters were evaluated in all groups. Histopathology of a full complement of tissues was evaluated in the control group as well as the high-dose caprenin group. No significant differences in body weight gain were measured with the balanced caloric diets, although feed conversion efficiency was reduced in the high-dose caprenin group. No adverse effects from the ingestion of caprenin were detected. The authors concluded that the results establish a no-observable-adverse-effect level (NOAEL) of more than 15% (w/w) caprenin in the diet (or more than 83% of total dietary fat), which is equal to a mean exposure level of more than 13.2 g/kg/day for male rats and more than 14.6 g/kg/day for female rats (Webb *et al.* 1993).

Dermal toxicity

In a subchronic study, no adverse effects were produced from topical application of myristic acid (C14) to rabbit skin. One-half ml of a 30 % preparation of myristic acid in ether and propylene glycol (solvents at a 1:1 ratio in concentration) was massaged into the depilated skin of the flanks of 5 rabbits daily for 30 days. The opposite flank of the rabbits was depilated and treated with solvent only. No significant macroscopic changes were observed. Microscopic lesions included thinning of collagen fibres in the superficial layer of the derm is after 10 days and a loose dermal infiltrate of lymphomononuclear cells and histocytes after 20 and 30 days (CIR, 1987).

A formulation "bath soap and detergent" containing 10-25% sodium stearate (C18) was used to conduct a dermal toxicity study in rabbits. Formulations at a dose of 2.0 g/kg were applied for 3 months to the skin by syringe daily, five days a week. No "untoward reactions" were observed (CIR, 1982).

Summary: The available data demonstrate the low toxicity of fatty acids and their salts, which is consistent with their long history of safe use in foods and the fact that many of the fatty acids are listed as GRAS.

5.2.1.5 Genetic Toxicity

In Vitro

Fatty acids are negative in *in vitro* bacterial systems used in the Ames test (BIBRA, 1988; BIBRA, 1996). In addition, saturated fatty acids up to and including C12, and the unsaturated acid C18:1, have shown inhibition of the mutagenic activity of N-nitrosodialkylamines on *Eschericha coli* (Negishi *et al.* 1984). Also, fatty acids from C12 up to C19 have shown anticlastogenic effects in the chromosome aberration test (Renner, 1986).

Capric acid (C10) produced negative results in the Ames test using *Salmonella typhimurium* strains TA97, TA98, TA100, TA1535 and TA1537 at concentrations ranging from 0-666 µg/plate, with and without metabolic activation (IUCLID, 2000c). It also produced negative results in the *Escherichia coli* reverse mutation assay without activation (IUCLID, 2000c).

Lauric acid (C12) has shown negative results in the Ames test using *Salmonella typhimurium* with and without metabolic activation at concentrations up to 2500 µg/plate. (IUCLID, 2000a).

Stearic acid (C18) was tested for mutagenicity using the Ames test with *Salmonella typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538. Spot tests were performed using 50 mg/ml stearic acid suspensions in distilled water (50 µg/plate) with and without microsomal activation from hepatic S9 fractions from rats induced with Aroclor 1254 (50 µl/plate). Stearic acid had no mutagenic activity over background in the strains tested with and without metabolic activation (CIR, 1987).

A solution of 99.9% pure oleic acid (C18) was tested in the Ames test using *Salmonella typhimurium* strains TA98, TA100 and TA1535. It was tested at concentrations of 1, 5, 10, 50, 100, 500, 1000 and 5000 µg/plate with and without metabolic activation and produced negative results (IUCLID, 2000e). In the *Escherichia coli* reverse mutation assay using *E. coli* strain WP2uvrA, concentrations of 1, 5, 10, 50, 100, 500 1,000 and 5,000 ug/plate, with and without activation, a solution of 99.9% pure oleic acid also produced negative results. It has also produced negative results in *Saccharomyces cerevisiae* and in DNA and damage repair assays using *Bacillus subtilis* (BIBRA, 1986; IUCLID, 2000e).

Fatty acids, C18-22 produced negative results with and without metabolic activation in the Ames test at concentrations ranging between 4-1250 µg/plate using *Salmonella typhimurium* (IUCLID, 2000g).

In Vivo

No *in vivo* mutagenicity data was located. However, there is no association between the normal intake of large amounts of fatty acids in the diet and mutagenicity. Therefore, the small increase via exposure to fatty acids and their salts in household cleaning products would also be considered not to increase the risk of mutagenicity.

Summary: Based on the available data which show lack of mutagenicity under in vitro conditions, fatty acids and their salts are not mutagenic.

5.2.1.6 Carcinogenicity

Numerous mechanisms for the role of dietary fat in tumourigenesis have been studied and reviewed (e.g. Welsch and Aylsworth, 1983; Diamond *et al.* 1980; Woutersen *et al. 1999*).

In a two year study by Hiasa *et al.* (1985), groups of 50 male and 50 female F344 rats, initially 7 weeks old, were given sodium oleate (C18) for 108-weeks at concentrations of 2.5 and 5.0% in the drinking water. Control rats were given distilled water only. Sodium oleate slightly reduced the body-weight gain in the males, but not in the females, while water consumption was slightly depressed in the females, but not in the males. A slight depression in serum bilirubin of males in the 5.0% group was the only statistically significant finding ($p<0.05$) in the serum and urine analyses and in the haematological determinations of treated and control groups.

In the groups given 5% sodium oleate, the mean weights of the liver of males and of the heart, pancreas and adrenals of females were significantly lower ($p<0.05$) than those of the respective controls, while the weight of the thymus in the females was significantly higher ($p<0.05$).

Tumours developed in various organs, but there was no significant difference between their incidence in oleate-treated and control rats, apart from the pancreatic tumours (0% - 0/41M, 1/43F; 2.5% - 4/40M, 1/39F; 5% - 7/45M, 1/45F). However, the incidence of pancreatic tumours was within the normal background level for this strain of rat and the result was attributed to the unusual absence of pancreatic tumours in the control rat. Based on a weight of evidence approach including consideration of the historical range of pancreatic tumours in these rats it was concluded that sodium oleate does not induce tumours when given orally to rats (Hiasa *at al.* 1985). *(Klimisch study rating – 2 i.e. reliable with restrictions)*

No evidence of carcinogenicity was seen in rats receiving 25% oleic acid (C18) in the diet (approximately 12.5 g/kg bodyweight per day) for 20 weeks (IUCLID, 2000e).

Also, due to their innocuous nature, fats and oils are commonly used as controls and as vehicles in animal toxicity studies. This along with the long history of safe use of the fatty acids and their salts, as well as the GRAS status for many of these chemicals, indicate no potential for carcinogenicity of these chemicals.

Summary: Based on the available data as well as the long history of safe use of these chemicals, it is not considered that the fatty acid salts possess carcinogenic activity, as a result of their use in household cleaning products.

5.2.1.7 Toxicity to Reproduction

15% oleic acid (C18) in the diet [approximately 7.5 g/kg bw/day] (the only dose tested) for 10 to 16 weeks did not affect the fertility of male rats but appeared to impair reproductive capacity in the females by interfering with parturition and mammary gland development. Mortality in the offspring was increased. No other information is available (BIBRA, 1986; IUCLID, 2000e).

Hendrich *et al.* (1993) conducted a study in which three generations of CBA/2 and C57Bl/6 mice were reared on semipurified diets containing 8.6% crude *Cuphea* oil. The *Cuphea* oil contained 76% capric acid (C10 fatty acid). Males of each generation were housed individually and fed for 13-weeks. Food intakes and body weights were measured weekly. Some males of each generation were fed for 5-12 months. Because *Cuphea* oil was in short supply, the F1 generation of the C57B1/6 strain were fed for 10 months, the F2 generation was fed for 8 months and the F3 generation was fed for 5 months; whereas in the CBA/2 strain, the F1 generation was fed for 11-12 months, the F2 generation was fed for 9-11 months and the F3 generation was fed for 6-8 months. The diet containing *Cuphea* oil did not impair reproductive parameters or cause any pathology in the mouse tissues examined. *Cuphea* oil moderately suppressed body weights and food intakes of mice in some groups between 4 and 13-weeks of age, but had no long-term effects on body weight, food intake or cholesterol status.

Again, the long history of safe use of these acids and their related glycerides and food oils, as well as the GRAS status for several of the fatty acids and their salts, indicate the low potential for reproductive toxicity of these chemicals.

Also, it is worth bearing in mind when considering the reproductive toxicity of fatty acids and their salts, that due to their innocuous nature, fats and oils are commonly used as controls and as vehicles in animal toxicity studies. For example, OECD Guideline 408 (repeated dose 90-day oral toxicity study in rodents) recommends the use of "a solution/emulsion in oil (e.g. corn oil)" as a vehicle where an aqueous vehicle is not suitable (OECD, 1993).

Summary: A three-generation reproductive study on a C10 fatty did not produce any reproductive effects. This along with the long history of safe use of the fatty acids indicate the low potential for reproductive toxicity of these chemicals.

5.2.1.8 Developmental Toxicity / Teratogenicity

Ishii *et al.* (1990) studied the effects of natural soap on the development of mouse embryos cultured *in vitro*. They found that there was no effect on embryo development at concentrations up to 0.05%. More than 0.05% natural soap gave rise to precipitates in the culture medium.

In a study by Palmer *et al.* (1975) 'soap' was examined for embryotoxic and teratogenic potential following percutaneous administration. Groups of rats and mice were treated with concentrations of 0.3, 3 and 30% of a standard soap solution. The formulated solutions were applied to the skin at the rate of 0.5 ml/rat or mouse per day with rats being dosed on days 2-15 and mice on days 2-13 of gestation. The concentrations of 0.3, 3 and 30% corresponded to nominal doses of 6, 60 and 600 mg/kg/day in rats and 50, 500, and 5000 mg/kg/day in mice.

In rats and mice treated with 30% soap solution the initial reaction consisted of erythema and oedema with peak response being attained by day 6 in mice and days 4 to 5 in rats. Clearly defined local reactions were not apparent at lower concentrations of soap. Weight loss, or marked retardation of bodyweight gain, reaching a peak at day 6 was observed for mice receiving soap at 3 or 30%. Rats were not conclusively affected by treatment as, even at the highest dose of 30%, weight gain was only slightly lower than that of controls. The marked reduction in numbers of litters containing viable young (due to non-pregnancy and/or total litter loss) recorded among mice treated with soap at 3 and 30% was considered secondary to maternal toxicity.

Effects on litter parameters were generally restricted to dosages causing marked maternal toxicity in mice, the principal effects being higher foetal loss (with consequent reduction in viable litter size) arising from an increased incidence of total litter loss. When dams showing total litter loss were excluded from the calculations, litter parameters were not unduly different from those of controls. At dosages that were non-toxic or only slightly toxic to the dam, litter parameters were not adversely affected as the only significant deviations from control values were in respect of the higher mean pup weights observed in rats at 0.3, 3 and 30% soap and the consequent higher litter weights at 0.3 or 30%. The incidences of major malformations, minor visceral or skeletal anomalies and skeletal variants were not statistically significant and produced no evidence of specific teratogenicity, even at maternally toxic dosages (Palmer *et al.* 1975).

It is important to bear in mind when considering the toxicity of fatty acids and their salts that due to their innocuous nature, fats and oils are commonly used as controls and as vehicles in animal toxicity studies. For example OECD Guideline 408 recommends the use of "a solution/emulsion in oil (e.g. corn oil)" where an aqueous vehicle is not suitable (OECD, 1993).

Summary: Available data do not provide evidence of significant developmental toxicity of fatty acid salts. Again, the long history of safe use of the fatty acids and their related glycerides and food oils, as well as the GRAS status for several members of the fatty acids and their salts, indicate the low potential for developmental toxicity of these chemicals.

5.2.1.9 Toxicokinetics

Fatty acids and their salts

Fatty acids are an endogenous part of every living cell and are an essential dietary requirement. They are absorbed, digested, and transported in animals and humans. Proposed mechanisms for fatty acid uptake by different tissues range from passive diffusion to facilitated diffusion or a combination of both (Abumrad *et al.* 1984; Harris *et al.*, 1980). Radioactivity from labelled fatty acids administered orally, intravenously, intraperitoneally, and intraduodenally has been found in various tissues and in blood and lymph (CIR, 1987).

Fatty acids taken up by the tissues can either be stored in the form of triglycerides (98% of which occurs in adipose tissue depots) or they can be oxidised for energy via the β-oxidation and tricarboxylic acid cycle pathways of catabolism (Masoro, 1977). The β-oxidation of fatty acids occurs in most vertebrate tissues utilising an enzyme complex for the series of oxidation and hydration reactions resulting in the cleavage of acetate groups as acetyl CoA. β-oxidation essentially reduces the alkyl chain length by 2 carbon atoms with the release of acetic acid. This leaves another carboxyl group on the shortened alkyl chain for subsequent further β-oxidation. An additional isomerisation reaction is required for the complete catabolism of oleic acid. Alternate oxidation pathways can be found in the liver (ω-oxidation) and the brain (α-oxidation) (CIR, 1987).

Long chain, saturated fatty acids are less readily absorbed than unsaturated or short chain acids. Stearic acid is the most poorly absorbed of the common fatty acids (Clayton & Clayton, 1982; Opdyke, 1979). Several investigators have also found increasing fatty acid chain length slightly decreased their digestibility (CIR, 1987).

Howes (1975) examined the turnover of [^{14}C] surfactants in the rat and found that at 6h after administration, the C10 and C12 soaps were readily metabolised and the main route of excretion was as $^{14}CO_2$. The C14 soap was readily incorporated into the body and the ^{14}C excretion was slow. The C16 and C18 soaps showed some metabolism with subsequent $^{14}CO_2$ excretion but most of the ^{14}C was recovered in the carcass at 6 hours.

Sodium

Sodium is an essential element in the diet but a high intake of sodium has been associated with cardio-vascular diseases. Sodium is readily absorbed throughout the small intestine and is subject to rapid exchange by the large majority of cells in the body. The main regulation of the body concentrations of sodium takes place in the kidney. The consumer exposure to household cleaning products results in negligible exposure to sodium (compared to dietary uptake) and therefore elevation of the amounts of sodium are not expected to occur as a result of exposure to fatty acid sodium salts in cleaning products or their residues.

Potassium

Potassium salts are generally readily absorbed from the gastro- intestinal tract. Potassium is excreted by the kidneys; it is secreted in the distal tubules in exchange for sodium or hydrogen ions. The capacity of the kidneys to conserve potassium is poor and urinary excretion of potassium continues even when there is severe depletion. Some potassium is excreted in the faeces and small amounts may also be present in saliva, sweat, bile, and pancreatic juice (Martindale, 1996). Again, exposure to cleaning products containing potassium salts will not increase the body burden of potassium.

Dermal Penetration

It has been shown that the greatest skin penetration of the human epidermis was with C_{10} and C_{12} soaps and the rate of percutaneous absorption of sodium laurate is greater than that of most other anionic surfactants. (Prottey and Ferguson, 1975; Madsen *et al.*, 2001; Howes, 1975).

Howes (1975) studied the percutaneous absorption of some anionic surfactants and showed that sodium decanoate was reportedly poorly absorbed through the skin of rats when in uncovered contact for 15 minutes. Penetration through excised human skin proceeded at a rate similar to that for excised rat skin for up to 6 hours; thereafter absorption through human skin was slightly quicker. Also, for the three soaps which penetrated the skin (C10, C12 and C14) there was a lag time of 1 hour before any measurable penetration occurred, but after this the rate of penetration steadily increased. Howes also calculated from human epidermal studies *in vitro* that only small amounts of the C10, C12 and C14 soaps would be likely to penetrate the skin from a 15 minute wash and rinse *in vivo*. The low penetration rates of the C16 and C18 soaps suggests that little or none of these would penetrate from a 15 minute wash and rinse *in vivo*.

5.2.2 Identification of critical endpoints

5.2.2.1 Overview on Hazard identification

Fatty acid salts are considered to be of low toxicity after oral and dermal exposure. The estimated LD50 for chemicals in this class is greater than 2,000 mg/kg via the oral route and greater than 3,000 mg/kg via the dermal route. The acute inhalation data are limited but this is not expected to be a significant route of exposure to these chemicals.

The skin and eye irritation potential of fatty acids and their salts is chain length dependent. Tests in animals and humans show that the irritation potential decreases with increasing chain length such that C12 is minimally irritant and the longer chain lengths, C14 and above, are not irritant.

The available data support the hypothesis that fatty acid salts are not skin sensitisers.

The available oral and dermal repeated dose toxicity studies demonstrate the low toxicity of fatty acids and their salts. This is consistent with the long history of safe use in foods for both fatty acids and glycerides. Further evidence of their safe use in foods is the Generally Recognised As Safe (GRAS) status of several of the fatty acids. Provided the cation (sodium or potassium) does not add excessively to the normal body load, which will not be the case following exposure to fatty acid salts in household cleaning products, then these substances are not considered hazardous.

Fatty acid salts are not considered to be mutagenic, genotoxic or carcinogenic, and are not expected to be reproductive or developmental toxicants, which again is consistent with their long history of safe use.

5.2.2.2 Rationale for identification of critical endpoints

Dermal exposure to fatty acid salts is the main exposure route for consumers using household cleaning products and subsequently, dermal effects such as skin irritation and sensitisation as well as long term dermal toxicity have to be considered with regard to the human risk assessment. A substantial amount of data are available addressing skin irritation and skin sensitisation potential for fatty acids and their salt solutions and fatty acid salts containing consumer product formulations. Dermal penetration studies have shown that soaps can penetrate the skin to varying extents and become available systemically and so the effects following long term exposure via the oral route have also been considered.

The eye irritation potential has to be considered, since accidental spillage may cause eye contact of fatty acid salts. For the assessment of accidental exposures via ingestion, the data on acute oral toxicity are considered.

5.2.2.3 Determination of NOAEL or quantitative evaluation of data

Considering the fact that the WHO felt it unnecessary to set an ADI for the salts of myristic, palmitic and stearic acids and since several of the fatty acids are listed as GRAS it was considered unnecessary to define a NOAEL that would be representative for the fatty acid salts as a group for use in the margin of exposure calculations.

5.3 Risk Assessment

5.3.1 Margin of Exposure Calculation

5.3.1.1 Exposure scenario: direct skin contact from hand washed laundry

From the exposure calculation (section 5.1.3.1), the dermal exposure to fatty acid salts as a result of hand washing was estimated to be 1.4×10^{-4} mg/kg body weight (0.1 µg/kg body weight). Given the fact that several of the fatty acids and their salts, including stearic acid, oleic acid and sodium palmitate are listed as GRAS, and since the WHO set an unlimited ADI for the salts of myristic, palmitic and stearic acids, it is not expected that the limited exposure to fatty acids salts from hand washing will result in any adverse effects.

As stated in Section 5.2.1.2, tests in animals and humans show that the skin irritation potential of fatty acid decreases with increasing length such that the longer chain lengths, C14 and above are not irritant and the existence of unsaturated carbon chains and carbon chain lengths of C16 to C18 contribute to a low skin irritation effect. As the majority of the carbon chain lengths of the soaps considered in this assessment were C12 and above (98.9%) and considering the relatively short contact time and low exposure, it is not expected that direct skin contact with fatty acid salts from hand washed laundry will cause irritation in consumers.

5.3.1.2 Exposure scenario: direct skin contact from contact via pretreatment of clothes

From the exposure calculation (section 5.1.3.1), the dermal exposure to fatty acid salts as a result of contact via pretreatment of clothes was estimated to be 2.0×10^{-3} mg/kg body weight (2.0 µg/kg body weight). As stated above, the fact that several of the fatty acids and their salts are listed as GRAS, and since the WHO set an unlimited ADI for the salts of myristic, palmitic and stearic acids, it is not expected that the limited exposure to fatty acids salts from laundry pretreatment will result in any adverse effects.

As stated above, the majority of the carbon chain lengths of the soaps considered in this assessment were C12 and above (98.9%) which have low skin irritation potential. Therefore, considering the relatively short contact time and low exposure, it is not expected that direct skin contact with fatty acid salts from pretreatment of clothes will cause irritation in consumers.

5.3.1.3 Exposure scenario: indirect skin contact from transfer from clothing

From the exposure calculation (section 5.1.3.1), the dermal exposure to fatty acid salts as a result of transfer from clothing was estimated to be 7.9×10^{-4} mg/kg body weight (0.79 µg/kg body weight). Given the fact that several of the fatty acids and their salts are listed as GRAS, and since the WHO set an unlimited ADI for the salts of myristic, palmitic and stearic acids, it is not expected that the limited exposure to fatty acids salts from hand washing will result in any adverse effects.

The majority of the carbon chain lengths of the soaps considered in this assessment were C12 and above (98.9%) which have low skin irritation potential. Therefore, considering the relatively short contact time and low exposure, it is not expected that indirect skin contact with fatty acid salts from transfer from clothing will cause irritation in consumers.

5.3.1.4 Exposure scenario: Inhalation of laundry powder dust & inhalation of sprays generated by aerosols

From the exposure calculation (section 5.1.3.1), the total inhalation exposure to fatty acid salts as a result of pouring washing powder into a machine and inhaling aerosols generated by spray cleaners was estimated to be 2.0×10^{-6} mg/kg body weight (0.002 µg/kg body weight).

Although the inhalation data on fatty acid salts are limited, given the low order of toxicity of these chemicals and the fact that the exposure is orders of magnitude below the general threshold of no concern of 1.5 μg /day as defined by Munro (1998), then inhalation exposure to fatty acids will not be a concern.

5.3.1.5 Exposure scenario: Accidental Exposure

The acute oral toxicity data for a range of fatty acid salts have shown that the LD50 is greater than 2000 mg/kg. This level of toxicity is generally considered as low. Based on such an LD50 value, the uptake of fatty acid salts must be extremely high to reach acute lethal effects. Although fatty acid salts have been used for a very long time in a variety of applications, acute cases of oral poisoning have not been reported in the literature. Therefore, it appears as if occasional accidental ingestion of a few milligrams of fatty acid salts or intentional overexposure to fatty acid salts via the oral route does not result in adverse effects, which is not surprising given the low toxicity profile of these chemicals.

The available information show that the skin and eye irritation potential of fatty acids and their salts decreases with increasing chain length, such that C12 is minimally irritant and the longer chain lengths C14 and above are not irritant. As 98.9% of the carbon chain length distribution for chemicals in this assessment consist of C12 chain lengths and above (see Section 3.4), the fatty acid salts used in household cleaning products will not induce skin or eye irritation following the limited exposure to the products containing these materials. Also, fatty acid salts do not induce skin sensitisation in those exposed. Nevertheless, eye and prolonged skin contact with neat products should be avoided as other surfactants present in the formulations could induce irritation effects. In the case of eye contact, immediate rinsing with plenty of water is also recommended. This immediate action has been shown in animal experiments to minimise irritation effects.

Considering the fact that soaps are almost completely removed from wastewater the exposure via drinking water is expected to be insignificant.

5.3.1.6 Exposure scenario: Total Consumer Exposure

In a worst case scenario, the consumer exposure from direct and indirect skin contact of neat or diluted fatty acid salts containing product, inhalation of laundry powder dust and spray cleaners containing fatty acid salts and from accidental ingestion, results in an estimated systemic fatty acid salt dose of 2.9 x 10^{-3} mg/kg (2.9 μg/kg) body weight per day.

Although many of the fatty acids and their salts are listed as GRAS and the WHO set an unlimited ADI for the salts of myristic, palmitic and stearic acids, in order to illustrate the large margin of exposure between exposure to fatty acid salts in household cleaning products and adverse effects, a margin of exposure can be calculated for fatty acids using a LOAEL of approximately 7500 mg/kg body weight per day for oleic acid (C18) (BIBRA, 1986), as representative of this group for systemic toxicity. This was from a dietary study in which the fertility of male rats was not affected, but the reproductive capacity of females did seem to be impaired and the morality in the offspring was increased. Using this LOAEL and applying an uncertainty factor of 10 to obtain a NOAEL, 750 mg/kg can be calculated as the NOAEL. Using this, the margin of exposure can be calculated as:-

MOE_{total}	**= systemic oral NOAEL / estimated total systemic dose**
	= 750 mg/kg bw per day / 2.9 x 10^{-3} mg/kg bw per day
MOE_{total}	**= 258,620**

5.3.2 Risk Characterisation

The detailed consideration of the different exposure scenarios for the handling and use of detergent products containing fatty acid salts did not reveal any risk for consumers from the use of these materials. The estimated human exposure to fatty acid salts shows a Margin of Exposure of 258,620. This is an extremely large margin of exposure and was calculated from the total exposure scenarios, which is an unrealistic situation and will be unlikely in an "in-use" situation, making the margin of exposure even more conservative.

The determined MOE is certainly large enough to be reassuring with regard to the relatively small variability of the hazard data on which it is based. The MOE is based on worst case exposure assumptions and the true consumer exposure is highly likely to be significantly lower than presented here.

In the UK, the Department of Health have set dietary reference values for fatty acids and recommend that total fatty acid intake should average 30 per cent of total dietary energy including alcohol (DoH, 1991). This equates to about 100 g of fatty acids per day or 1.7 g of fatty acids per kg body weight (1700 mg/kg body weight per day). The total consumer exposure to fatty acids and their salts from the use of household cleaning products was calculated to be 2.9 x 10^{-3} (0.0029 mg/kg) body weight per day. This exposure is several orders of magnitude below that which is recommended via the diet, further illustrating the point that exposure to fatty acid salts in household cleaning products does not pose any risk to consumers.

Despite the fact that this assessment was based largely on secondary data, it is clear from the extremely large MOE that further experimental data are not required.

The available toxicological information indicates that fatty acid salts are of low acute toxicity after oral and dermal exposure.

The skin and eye irritation potential of fatty acids and their salts is chain length dependent and decreases with increasing chain length. They are not skin sensitisers. The available oral and dermal repeated dose toxicity studies demonstrate the low toxicity of fatty acids and their salts. This is consistent with the long history of safe use in foods for both fatty acids and glycerides. Also, the fatty acid salts are not considered to be mutagenic, genotoxic or carcinogenic, and are not expected to be reproductive or developmental toxicants, which again is consistent with their long history of safe use.

Accidental ingestion of a fatty acid salt containing detergent product is not expected to result in any significant adverse health effect. This assessment is based on toxicological data demonstrating the low acute oral toxicity of fatty acid salts and the fact that not a single fatality has been reported in the UK, following accidental ingestion of detergents containing fatty acid salts.

In summary, the use of fatty acid salts in consumer products such as laundry and cleaning detergents does not raise any safety concerns with regard to systemic or local toxicity.

5.4 Discussion and Conclusions

Consumers are exposed to fatty acid salts through their presence in laundry and cleaning products mainly via the dermal route, and to a much lesser extent via the oral and inhalation routes. Skin exposure occurs mainly in hand-washed laundry, laundry pre-treatment and through fatty acid salt residues in the fabric after the washing cycle. Consumers may be orally exposed to fatty acid salts through accidental ingestion or via intentional over-exposure. The consumer aggregate exposure to fatty acid salts has been estimated to be 2.9×10^{-3} mg/kg (2.9 µg/kg) body weight per day.

The available toxicological data demonstrates that fatty acid salts are neither genotoxic, mutagenic or carcinogenic, nor was there any evidence of reproductive toxicity (except at very high exposure levels) or developmental or teratogenic effects in animals. In addition, the fatty acids and their salts have a long history of safe use in foods. Further evidence of their safe use in foods is the GRAS status of several of the fatty acids. The WHO also set an unlimited ADI for the salts of myristic, palmitic and stearic acids and stated that myristic, palmitic and stearic acid and their salts are normal products of the metabolism of fats. Their metabolic fate after absorption is well established. Provided the contribution of the cations does not add excessively to the normal body load, which would not be the case following exposure to fatty acid salts in household cleaning products, then there is no reason to consider these substances more hazardous than dietary fatty acids.

The comparison of the aggregate exposure from the various scenarios with a NOAEL from a study on oleic acid, results in a MOE of 258,620. The study used to derive the NOAEL is from a secondary source preventing its quality to be checked. Also, the study reported a LOAEL (not a NOAEL), for which an uncertainty factor of 10 was applied to calculate the NOAEL, and the study was conducted on oleic acid (a C18 chain length fatty acid) and may not be totally representative of this group of chemicals. However, it nonetheless illustrates the large MOE that exists between exposure to a member of this group of chemicals and any adverse effects they may cause. Further reassurance is provided by WHO's decision to set "an unlimited ADI" for the salts of a number of specified fatty acids, as outlined above.

In the UK, the recommended total fatty acid intake is about 100 g of fatty acids per day or 1.7 g of fatty acids per kg body weight (1700 mg/kg body weight per day), while the total consumer exposure to fatty acids and their salts from the use of household cleaning products was calculated to be 2.9×10^{-3} (0.003 mg/kg) body weight per day. This extremely large difference in exposure further highlights the fact that exposure to fatty acid salts in household cleaning products is of no concern to the consumer.

Based on normal habits and uses, the consumer exposure to fatty acid salts by inhalation, oral uptake and skin contact is negligible and therefore the associated risk is also negligible.

In summary, the human health risk assessment has demonstrated that the use of fatty acid salts in household laundry and cleaning detergents is safe and does not cause concern with regard to consumer use.

6. References

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IUCLID (2000e) IUCLID Dataset on Fatty acids, rape oil. Creation Date 19 February 2000. European Chemical Bureau, Ispra, Italy.

IUCLID (2000f) IUCLID Dataset on Fatty acids, C16-18 and C18-unsatd., sodium salts. Creation Date 19 February 2000. European Chemical Bureau, Ispra, Italy.

IUCLID (2000g) IUCLID Dataset on Fatty acids, C18-22. Creation Date 19 February 2000. European Chemical Bureau, Ispra, Italy.

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Appendix I

Physical and Chemical Properties for the Sodium Salts of C10-C22 Fatty Acids

Chainlength : C10

Molecular weight	194.3	[g.mol-1]	
Melting point	203	[°C]	SRC
Boiling point	485	[°C]	SRC
Vapour pressure at 25 [°C]	1.1×10^{-7}	[Pa]	SRC
Octanol-water partition coefficient	0.2	[log10]	SRC
Water solubility	31000	[mg.l-1]	SRC

Chainlength : C12

Molecular weight	222.3	[g.mol-1]	
Melting point	217	[°C]	SRC
Boiling point	508	[°C]	SRC
Vapour pressure at 25 [°C]	2.0×10^{-8}	[Pa]	SRC
Octanol-water partition coefficient	1.2	[log10]	SRC
Water solubility {measured at 24oC}	3200 {22000}	[mg.l-1]	SRC{1}

Chainlength : C14

Molecular weight	250.4	[g.mol-1]	
Melting point	227	[°C]	SRC
Boiling point	532	[°C]	SRC
Vapour pressure at 25 [°C]	3.9×10^{-9}	[Pa]	SRC
Octanol-water partition coefficient	2.2	[log10]	SRC
Water solubility	330	[mg.l-1]	SRC

Chainlength : C16

Molecular weight	278.4	[g.mol-1]	
Melting point	238	[°C]	SRC
Boiling point	555	[°C]	SRC
Vapour pressure at 25 [°C]	1.8×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	3.2	[log10]	SRC
Water solubility {measured at 20oC}	33{2000}	[mg.l-1]	SRC{1}

Chainlength : C18 (Stearate)

Molecular weight	306.4	[g.mol-1]	
Melting point	250	[°C]	MSDS
Boiling point	578.0	[°C]	SRC
Vapour pressure at 25 [°C]	1.3×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	4.1	[log10]	SRC
Water solubility (at 20oC)	3.3	[mg.l-1]	SRC

Chainlength : C18 (Oleate)

Molecular weight	304.5	[g.mol-1]	
Melting point	251	[°C]	MSDS
Boiling point	582	[°C]	SRC
Vapour pressure at 25 [°C]	1.7×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	3.9	[log10]	SRC
Water solubility {measured at 20oC}	5.2{50000}	[mg.l-1]	SRC {1}

Chainlength : C22

Molecular weight	362.6	[g.mol-1]	
Melting point	271	[°C]	SRC
Boiling point	624	[°C]	SRC
Vapour pressure at 25 [°C]	4.5×10^{-12}	[Pa]	SRC
Octanol-water partition coefficient	6.1	[log10]	SRC
Water solubility	0.032	[mg.l-1]	SRC

Data Sources:

SRC) SRC data are calculated by the EPIWIN programme, supplied by the Syracuse Research Corporation.

1) Stephen, H Stephen T (1963). Solubilities of inorganic and organic compounds. Pergamon Press, New York

Physical and Chemical Properties for the Potassium Salts of C10-C22 Fatty Acids

Chainlength : C10

Molecular weight	210.36	[g.mol-1]	
Melting point	203.31	[°C]	SRC
Boiling point	485.18	[°C]	SRC
Vapour pressure at 25 [°C]	1.13×10^{-7}	[Pa]	SRC
Octanol-water partition coefficient	0.2	[log10]	SRC
Water solubility	2.6×10^{4}	[mg.l-1]	SRC

Chainlength : C12

Molecular weight	238.41	[g.mol-1]	
Melting point	216.51	[°C]	SRC
Boiling point	508.38	[°C]	SRC
Vapour pressure at 25 [°C]	2.03×10^{-8}	[Pa]	SRC
Octanol-water partition coefficient	1.19	[log10]	SRC
Water solubility (at 24 °C)	2.7×10^{3}	[mg.l-1]	SRC

Chainlength : C14

Molecular weight	266.47	[g.mol-1]	
Melting point	227.36	[°C]	SRC
Boiling point	531.59	[°C]	SRC
Vapour pressure at 25 [°C]	3.87×10^{-9}	[Pa]	SRC
Octanol-water partition coefficient	2.17	[log10]	SRC
Water solubility	268.8	[mg.l-1]	SRC

Chainlength : C16

Molecular weight	294.52	[g.mol-1]	
Melting point	238.20	[°C]	SRC
Boiling point	554.80	[°C]	SRC
Vapour pressure at 25 [°C]	7.26×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	3.15	[log10]	SRC
Water solubility {measured at 20oC}	26.91	[mg.l-1]	SRC

Chainlength : C18 (Stearate)

Molecular weight	322.58	[g.mol-1]	
Melting point	294.04	[°C]	SRC
Boiling point	578.01	[°C]	SRC
Vapour pressure at 25 [°C]	1.34×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	4.13	[log10]	SRC
Water solubility {measured at 20 °C }	2.67	[mg.l-1]	SRC

Chainlength : C18 (Oleate)

Molecular weight	320.56	[g.mol-1]	
Melting point	250.71	[°C]	SRC
Boiling point	581.58	[°C]	SRC
Vapour pressure at 25 [°C]	1.04×10^{-10}	[Pa]	SRC
Octanol-water partition coefficient	3.92	[log10]	SRC
Water solubility {measured at 20 °C }	4.19	[mg.l-1]	SRC

Chainlength : C22

Molecular weight	378.69	[g.mol-1]	
Melting point	270.72	[°C]	SRC
Boiling point	624.42	[°C]	SRC
Vapour pressure at 25 [°C]	4.47×10^{-12}	[Pa]	SRC
Octanol-water partition coefficient	6.10	[log10]	SRC
Water solubility {measured at 20 °C }	0.02	[mg.l-1]	SRC

Data Sources:

SRC) SRC data are calculated b y the EP IWIN programme, supplied by the Syracuse Research Corporation.

Appendix II

Introduction

The following search strategy was used for an external literature search. This search was used alongside both internal searches and a data requ est spreadsheets sent to all relevant producer and formulator companies.

Table 1 - Chemicals used for data searching in HERA Fatty acid salts assessment:

Chemical Name	**Synonyms**	**Carbon Chain Length**	**CAS Number**
Decanoic acid, sodium salt**	Capric acid, sodium salt; sodium caprate	C10	1002-62-6
Dodecanoic acid*	Lauric acid	C12	143-07-7
Dodecanoic acid, sodium salt*	Lauric acid, sodium salt; Sodium laurate	C12	629-25-4
Tetradecanoic acid***	Myristic acid	C14	544-63-8
Tetradecanoic acid, sodium salt**	Myristic acid, sodium salt; Sodium myristate	C14	822-12-8
Hexadecanoic acid***	Palmitic acid	C16	57-10-3
Hexadecanoic acid, sodium salt**	Palmitic acid, sodium salt; Sodium palmitate	C16	408-35-5
Octadecanoic acid***	Stearic acid	C18	57-11-4
Octadecanoic acid, sodium salt*	Stearic acid, sodium salt; Sodium stearate	C18	822-16-2
9-Octadecanoic acid, potassium salt*	Oleic acid, potassium salt; Potassium oleate	C18	143-18-0
9-Octadecanoic acid, sodium salt*	Oleic acid, sodium salt; Sodium oleate	C18	143-19-1
9-Octadecanoic acid (Z-) cmpd with 2-aminoethanol (1:1)*	Monoethanolamine oleate	C20	2272-11-9
Fatty acids, C10-14***	--	C10-14	90990-09-3
Fatty acids, C12-18*	--	C12-18	67701-01-3
Fatty acids, C16-18*	--	C16-18	67701-03-5
Fatty acids, C14-18 and C16-18 unsat.d*	--	C16-18	67701-06-8
Chemical Name	Synonyms	Carbon Chain Length	CAS Number
Fatty acids, C14-22*	--	C14-22	68424-37-3
Fatty acids, C8-18 and C16-18 unsatd. Sodium salts*	--	C8-18	85408-69-1
Fatty acids, rape oil*	--	C22	85711-54-2

Note:-

*These chemicals are those which are used by the formulator companies (as provided to us by AISE)

**These chemicals are salts of fatty acids within the carbon chain lengths of interest to us, that may be useful for read across.

***The chemicals are fatty acids within the carbon chain length of interest to us and may be useful for read across data.

Keywords used in Search Strategy for Human Health Data

The following keyword s were used with each of the chem icals listed above in th e search strategy:-

HUMAN HEALTH

toxicity (or toxic?) cancer

carcinogen? (or carcinogenic/carcinogenicity) irritation

sensitisation teratogen? (or teratogenic/teratogenicity)

Developmental mutagen (or mutagenic/mutagenicity)

genotoxic? (or genotoxicity) reproduction

skin penetration Metabo lism

Excretion Absorption

ADME

ENVIRONMENTAL

Ecotoxicity/ Ecotoxicology/ Ecotoxicological Eco toxicity/ Eco toxicology/ Eco toxicological

Effects data Acute toxicity /aquatic and/or

LC50 / EC50 / IC50 with each of the following:

Algae Invertebrate

Daphnia Fish

Acute toxicity / terrestrial and/or

LC50 / EC50 / IC50 with each of the following:

Microorganism Earthworm

Plant Chronic toxicity / aquatic and/or

NOEC (No Observed Effect Concentration) with each of the following:

Algae Invertebrate

Daphnia Fish

Chronic toxicity / terrestrial and/or

NOEC (No Observed Effect Concentration) with each of the following:

Microorganism Earthworm

Plant Mesocosm

Bioaccumulation Fate

Biodegradation / ready / inherent / SCAS (Semi Continuous Activated Sludge) / Z ahn Wellens / MITI

Removal Degradation

Rate constants Aerobic

Anaerobic Abiotic

PHYSICAL – CHEMICAL

MW / Molecular Weight Mp / melting point

Bp / boiling point Vp / vapour pressure

Log P / log Kow / octanol water partition coefficient

Water solubility Koc – partition coefficient organic carbon water

Databases searched for Human health Data:

- IUCLID CD-ROM
- National Toxicology Program (NTP) website (http://ntp-server.niehs.nih.gov/)
- TOXNET website (http://toxnet.nlm.nih.gov/)

The TOXNET website contains links to the following databases:-

- Hazardous Substances Data bank (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB)
- TOXLINE abstrac ts database (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?TOXLINE)
- USEPA Integ rated Risk Information Sy stem (IRIS) database (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?IRIS.htm)

  - DART/ETIC (Developm ental and Reproductive toxicology) (http://toxnet.nlm.nih.gov/cgi-bin/sis/search)
  - GENE-TOX database (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?GENETOX)

- Pubmed abstracts database website (http://www4.ncbi.nlm.nih.gov/PubMed/)
- IPCS Environmental Health Criteria (EHC)
- International Agency for Research on Cancer (IARC) evaluations
- Joint Expert Committee on Food Additives (JECFA) evaluations
- BIBRA Toxicity profiles

Databases searched search sites for environmental effects and fate data:

- IUCLID CD-ROM
- http://rpssnt021.ps.u1889.unilever.com/cc_remedy_open/area_msds
- http://psu18.ps.u1889.unilever.com:8889/seac/owa/test
- http://www.epa.gov/ecotox/
- http://esc.syrres.com/efdb/TSCATS.htm
- http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB
- http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?TOXLINE.htm
- http://esc.syrres.com/efdb.htm
- http://wos.unilever.com/isicgi/CIW.cgi
- http://www.msdssolutions.com/en/
- http://library.dialog.com/bluesheets/html/bl0307.html
- http://physchem.ox.ac.uk/MSDS/#MSDS

Other search sites:

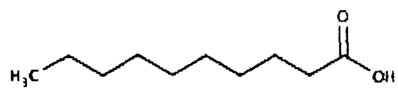
- BIOSIS previews (1969-present)
- Registry of Toxic Effects of Chemical Substances.

REFERENCE 4

SIS Home About Us Site Map & Search Contact Us
HSDB
▷ Env. Health & Toxicology ▷ TOXNET ▷ HSDB

DECANOIC ACID

CASRN: 334-48-5



For more information, search the NLM HSDB database.

Human Health Effects:

Human Toxicity Excerpts:

/HUMAN EXPOSURE STUDIES/ Capric acid produced no irritation when applied to human skin as a 1% solution in petrolatum for 48 hr in a closed-patch test. At higher concentrations (up to 1.0 M in propanol), the compound produced signs of irritation within 8 days in occlusive patch tests in human volunteers. No sensitization reactions were seen.
[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 737] **PEER REVIEWED**

/HUMAN EXPOSURE STUDIES/ /Decanoic acid was/ not sensitizing /to/ human. Five 48 hr covered applications of 1% decanoic acid in petrolatum were made over a 10 day period in 28 volunteers. None of them gave positive reactions when challenged 10 to 14 days after the induction phase with a final 48 hr closed patch test using 1% in petrolatum. /1% decanoic acid in petrolatum/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.32 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/HUMAN EXPOSURE STUDIES/ Daily /skin/ applications of 8.6% decanoic acid in propanol to 10 subjects caused irritation with reddening in 3 after 2 days and in 7 after 8 days.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.28 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/HUMAN EXPOSURE STUDIES/ Ten healthy male volunteers were exposed to 1.0 M sol of /decanoic acid on skin/ ... under occlusion for 10 days. /Decanoic acid/ produced an irritant response in all 10 subjects by the end of the test; no irritation had been evident on day 1 of the test. /Decanoic acid/ showed distinct cumulative irritation potential, but no acute irritation potential.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.28 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/HUMAN EXPOSURE STUDIES/ Solutions of decanoic acid were applied daily to /skin of/ 10 male volunteers for up to 10 days. 0.5 M capric acid caused an erythematous response in 7/10 volunteers within 8 days; 1.0 M decanoic acid caused a response in all 10 volunteers within 8 days.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.29 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/HUMAN EXPOSURE STUDIES/ ... Two laboratories conducted a direct comparison study of the acute irritation potential of three structurally related, undiluted fatty acids (octanoic acid, decanoic acid, and dodecanoic acid) in comparison to a benchmark positive control chemical (20% sodium dodecyl sulfate (SDS)). The studies were run within a 4-month period using the same commercial source of test chemicals. Test subjects were treated with each chemical under occluded patch conditions for gradually increasing exposure duration up to 4 hours. The results were then evaluated in terms of total cumulative incidence of positive responses and time response patterns. Using statistical comparisons of the proportion of the subjects with a positive irritant reaction to each substance, the rank order of irritation potential was decanoic acid > / = octanoic acid > SDS >> ... dodecanoic acid ...
[Robinson MK et al; Am J Contact Dermat 10(3):136-45 (1999)] **PEER REVIEWED** PubMed Abstract

/HUMAN EXPOSURE STUDIES/ A human maximization test was carried out on 28 volunteers. 1% concn ... caused no sensitization reactions. /1% concn/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.32 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/ALTERNATIVE and IN VITRO TESTS/ ... the highest concentrations of various fatty acids that are non-toxic to two human leukemic cell lines, Jurkat (T-lymphocyte) and Raji (B-lymphocyte) /were determined/. Toxicity was evaluated by either loss of membrane integrity and/or DNA fragmentation using flow cytometric analysis. There were no remarkable differences for the toxicity of the fatty acids between B and T cell lines. The cytotoxicity of the fatty acids was related to the carbon chain length and number of double bonds: docosahexaenoic acid=eicosapentaenoic acid=arachidonic acid=gamma-linolenic acid=stearic acid=palmitic acid > linoleic acid=palmitoleic acid > vacenic acid=lauric acid > oleic acid > elaidic acid > capric acid > butyric acid > caprylic acid=caproic acid=propionic acid.
[Lima TM et al; Toxicol In Vitro 16 (6): 741-7 (2002)] **PEER REVIEWED** PubMed Abstract

/ALTERNATIVE and IN VITRO TESTS/ The vasodilatory effects of various naturally occuring fatty acids (including decanoic acid) were investigated using human basilar and umbilical arteries. Test concn ranged from 4 uM to 4 mM. Decanoic acid was the most potent arterial relaxant. This was especially evident at 40 and 400 uM. The basilar artery was more responsive to decanoic acid than the umbilical artery (EC50 63 and 780 uM respectively). The relaxation was independent of endothelium, and was not related to the weak capacity of decanoic acid to inhibit Ca2+-induced contractions of K+-depolarized basilar arteries ...
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.42 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Human Toxicity Values:
EC50 Human (basilar artery) 63 uM; Effect: vasodilation.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.42 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

EC50 Human (umbilical artery) 780 uM; Effect: vasodilation.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.42 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Skin, Eye and Respiratory Irritations:
n-Decanoic acid was irritant to the skin of humans ... No skin sensitization was induced in volunteers treated with a dilute solution.
[British Industrial Biological Research Association (BIBRA) Working Group; BIBRA Toxicology International 6: (1996)] **PEER REVIEWED**

Probable Routes of Human Exposure:
NIOSH (NOES Survey 1981-1983) has statistically estimated that 7,879 workers (945 of these were female) were potentially exposed to decanoic acid in the US(1). Occupational exposure to decanoic acid may occur through inhalation and dermal contact with this compound at workplaces where decanoic acid is produced or used. Monitoring data indicate that the general population may be exposed to decanoic acid via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with this compound and other containing decanoic acid (SRC).

[(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available at http://www.cdc.gov/noes/ as of Jan 2008.] **PEER REVIEWED**

Body Burden:
Samples of mother's milk were collected from Bayonne, NJ; Jersey City, NJ; Pittsburgh, PA; Baton Rouge, LA; and Charleston, WV and analyzed for volatile and semivolatile organics. Decanoic acid was not detected(1).
[(1) Erickson MD et al; Acquisition and Chemical Analysis of Mother's Milk for Selected Toxic Substances. USEPA-560/13-80-029. Washington, DC: USEPA Off Pestic Toxic Subst pp. 152 (1980)] **PEER REVIEWED**

Average Daily Intake:
Fatty acids are an important part of the normal daily diet of mammals, birds and invertebrates.
[USEPA/OPPTS; R.E.D Facts. Soap Salts. Reregistration Eligibility Decisions (REDs) Database. EPA-738-F-92-013. Sept 1992. Available from the Database Query page at http://www.epa.gov/pesticides/reregistration/status.htm as of Sept 8, 2008.] **PEER REVIEWED**

Annual consumption is 18,833.33 lb. Individual consumption is 0.01596 mg/kg/day.
[Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 395] **PEER REVIEWED**

Emergency Medical Treatment:

Emergency Medical Treatment:

EMT Copyright Disclaimer:

The following Overview, *** NON-TOXIC INGESTION ***, is relevant for this HSDB record chemical.

Life Support:

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o   This overview assumes that basic life support measures
       have been instituted.
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Clinical Effects:

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0.2.1 SUMMARY OF EXPOSURE
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0.2.1.1 ACUTE EXPOSURE

A) USES: This document describes the management of substances generally considered nontoxic. Careful identification of the exact substance is critical for the appropriate application of the recommendations included in this document. These substances may still cause significant health effects due to idiosyncratic or allergic reactions, acting as a foreign body, or when the exposure is massive.

B) TOXICOLOGY: The most common effects are mucosal irritation or injury or gastrointestinal tract irritation.

C) EPIDEMIOLOGY: Ingestions of nontoxic substances are very common. More than mild effects suggest misidentification of the product or massive exposure.

D) WITH POISONING/EXPOSURE

1) The most common effects are mucosal irritation or injury or gastrointestinal tract irritation. Aspiration or upper airway obstruction from a foreign body are also possible.

0.2.23 OTHER

0.2.23.1 ACUTE EXPOSURE

A) A nontoxic ingestion occurs when the victim consumes an inedible product that usually does not produce symptoms. The importance of knowing that a product is nontoxic is that overtreatment is avoided and, more importantly, the victim and parents are not placed in the jeopardy of a panicky automobile ride to the physician or nearest hospital (Comstock, 1978).

B) Although some products may be labeled as nontoxic in this management, a patient can potentially have a non-dose-related life-threatening effect such as a hypersensitivity reaction to any substance, and be at risk of foreign body obstruction and aspiration (Kearney et al, 2006).

C) Materials referenced to this management have been considered very unlikely to produce any toxicity except in enormous doses. For example, ballpoint pen cartridges, even if sucked completely dry by a child, do not contain enough toxic materials to cause illness (Mofenson et al, 1984).

D) While almost anything, including water and table salt, may cause illness if taken in excessive amounts or by other than the normal route, normal exposures from these products would not be expected to produce toxicity (Horev & Cohen, 1994).

E) Some agents are harmful in manners different from that expected. A broken thermometer is dangerous not from the inert metallic mercury, but from the broken glass

(Mofenson et al, 1984). Most patients calling are more worried about mercury, which they think of as poison, than the glass.

F) General guidelines for determining whether an exposure can be categorized as nontoxic (reviewed in Weisman, 1998; (Mofenson et al, 1984):
  1) Absolute identification of the product, its ingredients, and its concentration.
  2) Absolute assurance that only the identified product was involved in the exposure.
  3) The exposure must be unintentional.
  4) "Signal words" identified by the Consumer Product Safety Commission (eg, Caution, Warning, Danger) must not be found on the label.
  5) A reliable approximation of the quantity of the substance involved in the exposure.
  6) The route of exposure can be assessed accurately from the patient's available history.
  7) Following the exposure, the patient is symptom-free.
  8) A follow-up consultation with the patient must be possible. In the case of a pediatric exposure, the parent must appear to be reliable.

Laboratory:

A) In general, laboratory testing is not needed. If the patient has more than mild symptoms, testing should be directed at evaluation of the symptoms.
B) Radiographs may be required to evaluate for retained objects, but many objects are not radio-opaque. Contrast studies may be used in some cases.
C) Patients with symptoms suggesting gastrointestinal obstruction or perforation should have CT scan imaging.

Treatment Overview:

0.4.2 ORAL EXPOSURE

A) MANAGEMENT OF MILD TO MODERATE TOXICITY
  1) Primarily supportive care. If the patient has oral irritation, they should rinse their mouth. Patients with persistent vomiting may require IV fluids.

B) MANAGEMENT OF SEVERE TOXICITY
  1) Severe toxicity suggests that the exposure was misidentified, idiosyncratic reactions (eg, allergic), or massive exposure. In these situations, management should be supportive and directed at the specific symptoms. Administer oxygen and obtain a chest radiograph if aspiration is suspected.

C) DECONTAMINATION
  1) Patients who have oral irritation should rinse their mouths with water.

D) AIRWAY MANAGEMENT

1) If a non-toxic substance has been aspirated or causes upper airway obstruction, airway management may be necessary.

E) ANTIDOTE

1) None

F) PATIENT DISPOSITION

1) HOME CRITERIA: Patients with exposure to a known non-toxic product and who have no more than mild symptoms may be managed at home.

2) OBSERVATION CRITERIA: Patients with self-harm ingestions or children in whom abuse or neglect are concerns should be referred to a healthcare facility for evaluation.

3) ADMISSION CRITERIA: Admission is almost never necessary unless aspiration or airway obstruction have occurred.

4) CONSULT CRITERIA: Toxicologist should be consulted if there is a question of possible systemic toxicity.

G) PITFALLS

1) Severe toxicity following exposure may suggest possible misidentification of the product.

0.4.3 INHALATION EXPOSURE

A) Although inhalation of common dust may not be considered toxic, it is certainly a hazard if there is inhalation of too many particles. Individuals should be removed from exposure to too high a concentration of even relatively nontoxic substances.

0.4.4 EYE EXPOSURE

A) Foreign materials in the eye may not cause a toxic reaction, but injury from a foreign body may occur. In such cases, the patient should be observed for eye irritation and should seek medical assistance if the irritation becomes significant.

0.4.5 DERMAL EXPOSURE

A) OVERVIEW

1) Foreign materials spilled on the skin may not represent a toxic or irritation hazard in small quantities but may produce adverse effects if applied in large quantities or if used over a significant period of time. Whenever possible, foreign materials should be removed from the skin with simple washing. Should skin irritation or erythema occur, a patient may wish to seek medical assistance.

Range of Toxicity:

A) These agents are considered not to be a toxic hazard in the quantities available through normal exposure or package size.

[Rumack BH POISINDEX(R) Information System Micromedex, Inc., Englewood, CO, 2013; CCIS Volume 156, edition expires May, 2013. Hall AH & Rumack BH (Eds): TOMES(R) Information System Micromedex, Inc., Englewood, CO, 2013; CCIS Volume 156, edition expires May, 2013.] **PEER

REVIEWED**

Antidote and Emergency Treatment:
/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Organic acids and related compounds/
[Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 176] **PEER REVIEWED**

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist respirations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Activated charcoal is not effective ... . Do not attempt to neutralize because of exothermic reaction. Cover skin burns with dry, sterile dressings after decontamination ... . /Organic acids and related compounds/
[Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 176-7] **PEER REVIEWED**

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Early intubation, at the first sign of upper airway obstruction, may be necessary. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Consider administering a beta agonist such as albuterol for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Organic acids and related compounds/
[Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 177] **PEER REVIEWED**

Animal Toxicity Studies:

Non-Human Toxicity Excerpts:
/LABORATORY ANIMALS: Acute Exposure/ ...RATED 9 ON RABBIT EYES. ...TESTED EXTERNALLY ON EYES OF RABBITS &...RATED NUMERICALLY ON SCALE OF 1-10 ACCORDING TO DEGREE OF INJURY...AFTER 24 HR /OBSERVATION/, PAYING PARTICULAR ATTENTION TO CONDITION OF CORNEA. MOST SEVERE INJURIES HAVE BEEN RATED 10.
[Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 1008] **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ The compound was a moderate to severe irritant when applied undiluted for 24 hr to intact or abraded rabbit skin in an occluded patch test. Capric acid (mixed isomers) produces severe corneal burns when applied as a 5 percent solution (0.5 ml in water or propylene glycol) to rabbit eyes, and was moderately irritating to rabbit skin in an open patch test. No deaths occurred in rats exposed for 8 hr to concentrated capric acid vapor.
[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 736] **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ A decanoic acid dose of 4.6 g/kg or more /adm orally/ caused excessive salivation and diarrhea /in rat/. At 10000 mg/kg, discharge from eyes and nose, some reduction of neuromuscular control and central nervous system depression were seen. No gross abnormalities were seen in lungs, kidneys, digestive tract and adrenals.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.22 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ Rats were exposed to saturated vapors of the mixed isomer of decanoic

acid. The maximum exposure time without any deaths occuring was 8 hr. /Mied isomer/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.23 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ Skin exposure to 500 mg /decanoic acid/ for 24 hr caused moderate irritation /in rabbit./
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.23 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ /Decanoic acid was/ highly irritating /to/ rabbit eyes. Instillation of 0.1 mL/tier neat material caused corneal clouding and moderate inflammation of the conjunctivae and iris. /Neat material/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.31 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ /Decanoic acid was/ not sensitizing /to/ guinea pig /in the/ Buehler test. One test group (20 animals) and one control group (10 animals) were used. For induction, a closed patch was applied for 6 hr once a wk for 3 wk. Two wk later, a challenge patch was applied for 6 hr (5% decanoic acid in acetone). Animals were examined at 24 and 48 hr. Result showed no sensitization in either group (0/20 and 0/10 for test and control groups, respectively). /5% decanoic acid in 40% w/w ethanol/'
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.31 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Acute Exposure/ Medium chain triglycerides (MCTs) are a family of triglycerides, containing predominantly, caprylic (C(8)) and capric (C(10)) fatty acids with lesser amounts of caproic (C(6)) and lauric (C(12)) fatty acids. MCTs are widely used for parenteral nutrition in individuals requiring supplemental nutrition and are being more widely used in foods, drugs and cosmetics. MCTs are essentially non-toxic in acute toxicity tests conducted in several species of animals. In ocular and dermal irritation testing MCTs exhibit virtually no potential as ocular or dermal irritants, even with prolonged eye or skin exposure. MCTs exhibit no capacity for induction of hypersensitivity.
[Traul KA et al; Food Chem Toxicol 38 (1): 79-98 (2000)] **PEER REVIEWED** PubMed Abstract

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Caprenin, a randomized triglyceride primarily comprising caprylic (C8:0), capric (C10:0), and behenic (C22:0) acids, was administered in a semi-purified diet to weanling Sprague-Dawley rats (25/sex/group) at dose levels of 5.23, 10.23 or 15.00% (w/w) for 91 days. Corn oil was added at 8.96, 5.91 and 3.00%, respectively, to provide essential fatty acids and digestible fat calories. Corn oil alone (12.14%) and a blend of medium-chain triglyceride (MCT) oil plus corn oil (11.21 and 3.13%, respectively) served as controls. All diets were formulated to provide about 4000 kcal/kg of diet and 26.8% of digestible calories from fat by assuming that corn oil, MCT oil, and caprenin provided 9, 7 and 5 kcal/g, respectively. Survival, clinical signs, body weight, feed consumption, feed efficiency, organ weights, organ-to-body-weight ratios, organ-to-brain-weight ratios, haematological values and clinical chemistry parameters were evaluated in all groups. Histopathology of a full complement of tissues was evaluated in the corn oil and MCT oil control groups as well as the high-dose caprenin group. Additional rats (n = 5/sex/group) were included in the study to determine whether there was marked storage of C22:0 in heart, liver or perirenal fat at the end of the 91-day feeding period. No significant differences in body weight gain were measured with the balanced caloric diets, although feed conversion efficiency was reduced in the high-dose caprenin group. No adverse effects from the ingestion of caprenin were detected, nor were significant amounts of C22:0 present in the fat extracted from the selected fat depot sites. These results establish a no-observable-adverse-effect level (NOAEL) of more than 15% (w/w) caprenin in the diet (or more than 83% of total dietary fat), which is equal to a mean exposure level of more than 13.2 g/kg/day for male rats and more than 14.6 g/kg/day for female rats.
[Webb DR et al; Food Chem Toxicol. 31 (12): 935-46 (1993)] **PEER REVIEWED** PubMed Abstract

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Medium chain triglycerides (MCTs) are a family of triglycerides, containing predominantly, caprylic (C(8)) and capric (C(10)) fatty acids with lesser amounts of caproic (C(6)) and lauric (C(12)) fatty acids. ... Ninety-day toxicity tests did not result in notable toxicity, whether the product was administered in the diet up to 9,375 mg/kg body weight/day or by intramuscular (im) injection (up to 0. 5 mL/kg/day, rabbits).
[Traul KA et al; Food Chem Toxicol 38 (1): 79-98 (2000)] **PEER REVIEWED** PubMed Abstract

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ No gastric lesions were evident in rats fed capric acid (10 percent in diet) for 150 days.

[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 736] **PEER REVIEWED**

/LABORATORY ANIMALS: Chronic Exposure or Carcinogenicity/ 15 male and 15 female /Wistar/ rats were fed the /40% medium chain / triglyceride (MCT) diet daily for 47 wk. Blood samples, weight gain and fecal samples were taken/analyzed during the experimental phase. Organ weights were taken at necropsy, and limited microscopic analysis was performed. Various organs and the carcass were analyzed for fat content. No adverse effects were observed. Fat deposition was lower than might be expected on normal fat diets. /MCT contained 21% decanoic acid./
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.35 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ 12 wk old McCollum-Wisconsin rats were fed diets containing medium chain triglyceride (MCT, unspecified level). Three wk later the rats were mated. The F1 offspring were fed on normal diet for 12 wk, and then fed the same MCT diet, and mated 3 wk later. There were no adverse effects on the F1 litter size or birthweight. Milk secretion of the F1 rats was significantly reduced. There was also a higher mortality (20 to 22%) during lactation for the F2 group fed the MCT diet. /MCT contained 25% decanoic acid./
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.38 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Capric acid administered daily (37 mg/kg) to pregnant rabbits increased sensitivity to oxytocin-induced labor.
[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 736] **PEER REVIEWED**

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Medium chain triglycerides (MCTs) are a family of triglycerides, containing predominantly, caprylic (C(8)) and capric (C(10)) fatty acids with lesser amounts of caproic (C(6)) and lauric (C(12)) fatty acids. ... There was no evidence that intravenous (iv) or dietary administration of MCTs adversely affected the reproductive performance of rats or resulted in maternal toxicity, fetal toxicity or teratogenic effects at doses up to 4.28 g/kg body weight/day (iv) or 12,500 mg/kg body weight/day (dietary). There was no evidence that dietary administration of MCTs adversely affected the reproductive performance of pigs or resulted in maternal toxicity, fetal toxicity or teratogenic effects at doses up to 4000 mg/kg body weight/day in the diet. In rabbits, following iv administration, the maternal and fetal no-observed-adverse-effect levels (NOAELs) were between 1.0 and 4.28 g/kg body weight/ day. ...
[Traul KA et al; Food Chem Toxicol 38 (1): 79-98 (2000)] **PEER REVIEWED** PubMed Abstract

/ALTERNATIVE and IN VITRO TESTS/ OCTANOIC ACID (100 MILLIMOLES) & DECANOIC ACID (10 MILLIMOLES) INDUCED CONTRACTURES IN ISOLATED FROG & RAT MUSCLES AFTER 20-30 MIN EXPOSURE.
[KOESSLER F, KUECHLER G; ACTA BIOL MED GER 36 (7-8) 1085-95 (1977)] **PEER REVIEWED**

/ALTERNATIVE and IN VITRO TESTS/ Decanoic acid was highly toxic to the eggs of the amphibian Triturus helveticus. A saturated (0.1M) soln caused cytolysis within 1 hr.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.39 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/ALTERNATIVE and IN VITRO TESTS/ A prokaryote (the cell wall-less microbe Acholeplasma laidlawii) and an eukaryote (the human B-cell line F4) were exposed to decanoic acid ... /Decanoic acid/ caused cytolysis and cytotoxicity to both cell types, depending on the concn used. At 0.5 mM ... decanoic acid no effects were observed, but higher concn were lethal. It appeared that a membrane target was involved.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.43 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/GENOTOXICITY/ In Ames tests, decanoic acid (0 to 666 ug/plate) gave negative results in Salmonella typhimurium strain TA 97, TA 98, TA 100, TA 1535, and TA 1537 with or without metabolic activation.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.37 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/GENOTOXICITY/ In an Escherichia coli reverse mutation assay, decanoic acid was applied to agar plates innoculated with various concn of E. coli strain Sd-4-73 (streptomycin dependent). Decanoic acid was either applied directly to the agar or on filter paper disc. Decanoic acid was reported as having no mutagenic activity.

[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.37 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Ecotoxicity Excerpts:

/OTHER TERRESTRIAL SPECIES/ Of 11 C6-22 even-numbered saturated and unsaturated fatty acids and their potassium salts tested for toxicity to balsam woolly aphid (Adelges piceae), the most effective fatty acids were capric acid (C10 saturated) and oleic acid (C18 unsaturated).
[Puritch GS; Can J For Res 5 (4): 515-22 (1975)] **PEER REVIEWED**

/OTHER TERRESTRIAL SPECIES/ /The decanoic acid/ concn that immobilizes 95% of the nematodes (Panagrellus redivivus) within 1 hr (ED95) is 156 ppm.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.20 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/OTHER TERRESTRIAL SPECIES/ The toxicity of ... /decanoic acid was/ evaluated using rice bloodworm larvae (10 larvae each group). Mortality was assessed after 24 hr exposure to 1, 10, 50 mg/L ... Decanoic acid caused 100% mortality at 10 or 50 mg/L; at 1 mg/L it caused 12 to 15% mortality.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.23 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/OTHER TERRESTRIAL SPECIES/ The insecticidal property of ... /decanoic acid/ was examined in 2 Drosophila species (D. mojavensis and D. nigrospiracula), using 2 cacti (agria and organpipe) as food source. Triplicate groups of 50 larvae were exposed to each food source, and given 30 days to emerge into adults. Decanoic acid (0.5% and 1.0%) was lethal to all D. nigrospiracula larvae. D. mojavensis was more tolerant, with viabilities of 76% and 9.3% at 0.5% and 1.0% decanoic acid respectively. Viability was 83 to 86% in the controls.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.44 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/OTHER TOXICITY INFORMATION/ The minimal growth-inhibitory amount of decanoate stopped growth, respiration, adenosine 5'-triphosphate synthesis, and amino acid transport of Bacillus subtilis in a culture containing amino acids and citrate as carbon sources. /Decanoate/
[Levin BC, Freese E; Antimicrob Agents Chemother 12 (3): 357-67 (1977)] **PEER REVIEWED** PubMed Abstract

/OTHER TOXICITY INFORMATION/ Bacillus megaterium /was exposed to decanoic acid/ for 24 hr at 25 deg C in nutrient broth. Ethanol /was used/ as solvent. Minimum inhibitory concn (MIC) is 1 mmol (172.26 mg)/L.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.18 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/OTHER TOXICITY INFORMATION/ Vibrio parahaemolyticus (bacterium) /was exposed to decanoic acid/ for 9 hr at 30 deg C in complex medium. Ethanol /was used/ as solvent. Minimum inhibitory concn (MIC) for arithmetic difference between percentage transmittance (620 nm) of control (ethanol only) and test cultures is 60 mg/L.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.19 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/OTHER TOXICITY INFORMATION/ ... Decanoic acid had strong fungicidal activity towards Aspergillus niger, Penicillium citrinum, Candida utilis and Saccharomyces cerevisiae.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.43 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Non-Human Toxicity Values:

LD50 Rat oral 3320 mg/kg
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.22 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LD50 Rat oral 3730 mg/kg /mix isomers/

[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.23 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LD50 Rat oral 15800 mg/kg /5% decanoic acid in 40% w/w ethanol/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.23 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LD50 Mouse iv 129 mg/kg
[Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1075] **PEER REVIEWED**

LD50 Rabbit dermal >5000 mg/kg
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.24 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LD50 Rabbit dermal 1.77 mL/kg /Mix isomer/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.24 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Ecotoxicity Values:
LC50; Species: Xenopus laevis (African clawed frog, embryo); Conditions: freshwater, renewal, pH 7.0-7.8; Concentration: 24000 ug/L for 96 hr (23000-25000 ug/L) /> or =98% purity/
[Dawson DA et al; Teratog Carcinog Mutagen 16 (2): 109-24 (1995) Available from, as of December 27, 2007: http://cfpub.epa.gov/ecotox/quick_query.htm **PEER REVIEWED**

EC50; Species: Xenopus laevis (African clawed frog, embryo); Conditions: freshwater, renewal, pH 7.0-7.8; Concentration: 7500 ug/L for 96 hr (7000-9000 ug/L); Effect: increased developmental changes, general (craniofacial defects, abnormal gut coiling) /> or =98% purity/
[Dawson DA et al; Teratog Carcinog Mutagen 16 (2): 109-24 (1995) Available from, as of December 27, 2007: http://cfpub.epa.gov/ecotox/quick_query.htm **PEER REVIEWED**

LC50 Oryzias latipes (Red Killifish) 31 mg/L/96 hr /In seawater; other conditions of bioassay not specified/
[Verschueren, K. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold Co., 1996., p. 405] **PEER REVIEWED**

LC50 Oryzias latipes (Red Killifish) 20 mg/L/96 hr /In freshwater; other conditions of bioassay not specified/
[Verschueren, K. Handbook of Environmental Data on Organic Chemicals. 3rd ed. New York, NY: Van Nostrand Reinhold Co., 1996., p. 405] **PEER REVIEWED**

LC50 Oryzias latipes (red killifish) 54 mg/L/96 hr; Conditions: semistatic, freshwater (renewal every 24 hr), 25 + / - 2 deg C, pH 7.2 /Sodium salt/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.15 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LC50 Oryzias latipes (red killifish) 31 mg/L/48 hr; Conditions: seawater test, salinity 30 ppt, 25 + / - 2 deg C, pH 8.2
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.15 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

LC50 Leuciscus idus (golden orfe) 95 mg/L/48 hr /Conditions of bioassay not specified in source examined/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.15 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

EC50 Nitzschia closterium (marine diatom) 0.002 mmol (0.3 mg)/L/72 hr; Conditions: natural seawater; Effect: cell growth measured spectrophotometrically
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.17 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

EC50 Bacillus subtilis (bacterium) 0.25 mmol (43.1 mg)/L/60 min; Conditions: complex medium, 37 deg C, ethanol as solvent (final concn < 1%); Effect: inhibition of rate of duplication
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.18 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

EC50 Methanothrix sp (bacterium) 5.9 mmol (1016 mg)/L/24 hr; Conditions: Upflow anaerobic sludge bed rector (predominant methanogen in sludge: Methanothrix), 30 deg C, pH 7; Effect: inhibition of acetoclastic methanogenic activity
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.19 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Ongoing Test Status:
European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) (2000 CD-ROM edition). Available from the Database Query page at: http://ecb.jrc.it/esis/esis.php as of January 23, 2008.
UNREVIEWED

Metabolism/Pharmacokinetics:

Metabolism/Metabolites:
The rate of intestinal absorption and hepatic uptake of medium chain fatty acids (MCFA) was investigated in 6 pigs. The pigs were fitted with a permanent fistula in the duodenum, and catheters in the portal vein, carotid artery and hepatic vein. Decanoic acid (esterified with octanoic acid) was infused into the duodenum for 1 hr. regular blood samples were taken over 12 hr and analysed for non-esterified decanoic acid content ... The amt of non-esterified MCFA taken up per hr by the liver were close to those absorbed from the gut via the portal vein, showing that the liver is the main site of MCFA metabolism in pigs. /Decanoic acid esterified with octanoic acid as medium-chain triacylglycerols/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.40 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Capric acid is metabolized by the 13-oxidative pathway, giving rise to C8- and C6-dicarboxylic acids (suberic and adipic acids) in rats. Capric acid metabolism also produced ketone bodies in rats, rabbits, dogs, piglets, and goats. Activation of lipid metabolism by starvation, fat-feeding, and experimental diabetes increased the extent of ketosis in rats. omega-Oxidation, leading to the excretion of sebacic acid, and chain elongation reactions have been reported. Metabolism of capric acid is rapid; in humans given [1-14C]decanoic acid orally, about 52% of the radioactivity was recovered within 2.5 to 4 hr.
[Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 736] **PEER REVIEWED**

(14)C-labelled fatty acids (including 240 mg decanoic acid) were fed by intubation into lactating rabbits. The animals were killed 24 hr later, and the mammary gland lipids were analyzed. Decanoic acid was extensively metabolized. Resynthesis after degradation to C2 units led to uniform alternate labelling in the C2-C10 acids, whereas C12-C18 acids had an excess of (14)C at the carboxyl end. Acids formed by beta-oxidation down to C12 (but not below) were also present in the mammary gland lipids.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.41 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Absorption, Distribution & Excretion:
The rate of intestinal absorption and hepatic uptake of medium chain fatty acids (MCFA) was investigated in 6 pigs. The pigs were fitted with a permanent fistula in the duodenum, and catheters in the portal vein, carotid artery and hepatic vein. Decanoic acid (esterified with octanoic acid) was infused into the duodenum for 1 hr. Regular blood samples were taken over 12 hr and analysed for non-esterified decanoic acid content. Decanoic acid levels in portal vein blood rose sharply after the beginning of the infusion (confirming data previously reported for dogs and rats), and showed a bi-phasic time course with 2 maximum values (at 15 min and 75 to 90 min). 54% of the decanoic acid was recovered in portal blood samples. The amt of non-esterified MCFA taken up per hr by the liver were close to those absorbed from the gut via the portal vein, showing that the liver is the main site of MCFA metabolism in pigs. /Decanoic acid esterified with octanoic acid as medium-chain triacylglycerols/

[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.40 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The influence of pancreatic enzyme secretion on the intestinal absorption of medium-chain fatty acids (MCFA) was investigated in 3 pigs. The pancreatic ducts were ligated (so producing exocrine pancreatic deficiency) and fitted with a permanent fistula, and catheters fitted in the portal vein and carotid artery. The decanoic acid triacylglycerol mixture was infused into the duodenum for 1 hr. Blood samples were taken over 8 hr and analysed for non-esterified decanoic acid content. Decanoic acid level incr slowly after the start of the infusion, reaching a max after 90 to 120 min. This contrasts with previous studies ... where healthy pigs reached a max blood concn after 15 min. This indicates that pancreatic lipase activity is not the pathway for de-esterification of MCFA. 27% of the decanoic acid was recovered from the portal blood flow. This is lower than seen previously, but confirms that more than one pathway is involved as decanoic acid production was not completely suppressed. /Decanoic acid esterified with octanoic acid as medium-chain triacylglycerols/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.41 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The influence of triglyceride structure on intestinal absorption was investigated. The triglycerides were composed of octanoic (C8), decanoic (C10) and linoleic (C18:2) acids (either as a structured oil, with the C8 and C10 at the sn-1 and sn-3 positions, or as a randomized oil, with the 3 acids in a random distribution). Absorption of the 3 acids varied; absorption of the C18:2 was highest from the structured oil, when it occupied the sn-2 position. Absorption of the 2 shorter chain fatty acids was highest from the randomized oil, when both acids occupied the sn-2 position approximately 33% of the time.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.31 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

(14)C-labelled fatty acids (including 240 mg decanoic acid) were fed by intubation into lactating rabbits. The animals were killed 24 hr later, and the mammary gland lipids were analyzed. Decanoic acid was extensively metabolized. Resynthesis after degradation to C2 units led to uniform alternate labelling in the C2-C10 acids, whereas C12-C18 acids had an excess of (14)C at the carboxyl end. Acids formed by beta-oxidation down to C12 (but not below) were also present in the mammary gland lipids.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.41 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Intestinal absorption of /(3)H-/labelled fatty acids (including decanoic acid) was investigated in the rat. The common bile and pancreatic duct was diverted, and a loop of the duodenum cannulated 24 hr later. The lipid mixture was introduced into each experimental loop, and the loop was then removed within the next 15 min. Radioactivity distribution studies confirmed that these fatty acids are absorbed in their non-esterified form, and that they are absorbed much more rapidly than oleic acid. Auto radiographic studies showed that the medium chain fatty acids are taken up in a molecular or aggregate form, leave the epithelial cells by way of the lateral plasma membrane, and are then found in the blood capillaries.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.42 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

... Decanoic acid is very lipid sol; a log octanol/water partition coefficient of 4.09 is reported. This indicates that decanoic acid has the potential to transfer to breast milk ...
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.44 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The permeability of the blood-brain barrier to ... (14)C-labelled /decanoic acid/ was studied by injecting ... /decanoic acid/ into common carotid artery of rats, and decapitating the rat 15 sec later ... the uptake of decanoic acid was 88%.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.45 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Children who suffer from seizures which are not controllable by drugs have apparently been successfully treated with MCT (medium chain triglyceride) diet. The MDT diet is an emulsion containing primarily (81%) octanoic acid, but also contains 15% decanoic acid. In this study 15 children were receiving 50 to 60% of their energy requirement s from the MCT emulsion. Blood samples were analyzed for decanoic and octanoic acid levels. There was a wide variation in absolute levels, possibly due to poor patient compliance, but all patients showed low levels

in the mornings, rising to high levels in the evenings. This suggested that both acids are rapidly metabolized. /Medium chain triglyceride/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.45 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Mechanism of Action:
It has been shown that polyunsaturated fatty acids such as arachidonic and docosahexanoic acids but not monounsaturated and saturated long-chain fatty acids promote basal and nerve growth factor (NGF)-induced neurite extension of PC12 cells, a line derived from a rat pheochromocytoma. On the other hand, short-chain fatty acids and valproic acid (2-propylpentanoic acid) enhance the growth of neurite processes of the cells only in the presence of inducers. In this study, /investigators/ demonstrated that straight medium-chain fatty acids (MCFAs) at millimolar concentrations alone potently induced neuronal differentiation of PC12 cells. ... Nonanoic, decanoic, and dodecanoic acids also induced growth of neurite processes, but their maximal effects were less marked than that of octanoic acid. ...
[Kamata Y et al; Neuroscience 146 (3): 1073-81 (2007)] **PEER REVIEWED** PubMed Abstract

... the effect of fatty acids on interleukin (IL)-8 production in a human intestinal epithelial cell line (Caco-2) /was investigated/. The cells were cultured as monolayers on microporous membranes in culture inserts. Oleic acid (OA), capric acid (CA), docosahexaenoic acid (DHA) and eicosapentaenoic acid (EPA) were applied to the apical compartment of Caco-2 cell monolayers. The concentration of IL-8 in the basolateral medium was measured by using enzyme-linked immunosorbent assay, and the expression of IL-8 mRNA was measured by using competitive reverse transcription--polymerase chain reaction. Protein kinase C inhibitors (GF109203X and calphostin C) and H-7 (a protein kinase inhibitor) were used to study the mechanisms by which IL-8 production is stimulated. Both OA and CA enhanced IL-8 production (approximately fivefold), whereas DHA and EPA did not. Both OA and CA also enhanced IL-1-induced IL-8 production. The onset of OA-induced IL-8 production was delayed compared with that of CA-induced IL-8 production. Both OA and CA enhanced IL-8 mRNA expression (approximately fivefold) after 6 and 3 hr, respectively. The protein kinase inhibitor (H-7) reduced both OA- and CA-induced IL-8 production by 88.0 and 85.9%, respectively. The protein kinase C inhibitors (GF109203X and calphostin C) reduced OA-induced IL-8 production by 29.3 and 54.5%, respectively, but showed no effect on CA-induced IL-8 production. These findings suggest that not only OA but also CA stimulates IL-8 production in intestinal epithelial cells, and the mechanisms of action differ between OA and CA.
[Tanaka S et al; J Gastroenterol Hepatol 16 (7): 748-54 (2001)] **PEER REVIEWED** PubMed Abstract

Interactions:
The effects of sodium caprate and sodium caprylate on transcellular permeation routes were examined in rats. The release of membrane phospholipids was significantly increased only by caprate, while protein release did not change from the control in the presence of caprate or caprylate, indicating that the extent of membrane disruption was insufficient to account for the extent of the enhanced permeation. Using brush border membrane vesicles prepared from colon, with their protein and lipid component labeled by fluorescent probes, the perturbing actions of caprate and caprylate toward the membrane were examined by fluorescence polarization. Caprate interacted with membrane protein and lipids, and caprylate mainly with protein, causing perturbation to the membrane. The release of 5(6)-carboxyfluorescein previously included in brush border membrane vesicles was increased by caprate but not by caprylate. These results suggest that caprate enhances permeability via the transcellular route through membrane perturbation. /Sodium caprate/
[Tomita M et al; Pharm Res 5 (12): 786-9 (1988)] **PEER REVIEWED** PubMed Abstract

Skin permeation rates were measured in vitro using human skin samples. 6 model cmpd of diverse physicochemical properties were dissolved in propylene glycol, and the permeation rates studied in the presence and absence of various fatty acids (including decanoic and neodecanoic acid). Both decanoic and neodecanoic acid increased the skin diffusivity of 4 of the 6 model cmpd, but only decanoic acid incr the permeation rate of propylene glycol ...
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.39 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The in vitro human skin permeation rate of an analgesic (buprenorphine) was incr by a factor of 3.5 by the addition of 0.5% decanoic acid.
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The enhancing action of decanoic acid on the intestinal absorption of phenosulfonphthalein (PSP) was studied in rats. Decanoic acid and 2 hydroxy derivatives enhanced PSP absorption to varying degrees; PSP was no longer absorbed once the enhancer had been completely absorbed. Absorption enhancement correlated with the ability to sequester calcium ions.
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Sodium caprate incr the epithelial permeability of PEG 4000 by 3.5 times in culture Caco-2 cells. This correlated with previous in vivo experiments with rat jejunum and colon in situ. PEG 4000 is poorly absorbed on its own. The absorption enhancing effect of sodium caprate was unchanged in the absence of mucosal Ca2+ chelation. /Sodium caprate/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.40 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The vasodilatory effects of various naturally occuring fatty acids (including decanoic acid) were investigated using human basilar and umbilical arteries. Test concn ranged from 4 uM to 4 mM. Decanoic acid was the most potent arterial relaxant. This was especially evident at 40 and 400 uM. The basilar artery was more responsive to decanoic acid than the umbilical artery (EC50 63 and 780 uM respectively). The relaxation was independent of endothelium, and was not related to the weak capacity of decanoic acid to inhibit Ca2+-induced contractions of K+-depolarized basilar arteries. Decanoic acid also inhibited contractions elicited by KCl, serotonin and the thromboxane analogue U46619.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.42 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

The effects of saturated straight-chain fatty acids with chain lengths of C8-C18 on the permeation of indomethacin and 6-carboxyfluorescein through rat skin were studied in vitro; the relationship between enhancing effects of the fatty acids and disordering of stratum corneum lipid domains was also determined. The largest enhancement in the permeation of both drugs was obtained with dodecanoic acid (lauric acid). Except for capric acid (C10), the permeation enhancing effects of the fatty acids were related to the perturbation increase of lipid domain in the stratum corneum. Capric acid appeared to enhance drug permeation by separate mechanisms. The uptake of fatty acids into stratum corneum was not related to permeation enhancing effects. It was concluded that, except for capric acid, the penetration enhancing effects of a series of fatty acids (C8-C18) are related to the perturbation increase of lipid domain in stratum corneum.
[Morimoto K et al; Drug Dev Ind Pharm 21 (17): 1999-2012 (1995)] **PEER REVIEWED**

Pharmacology:

Therapeutic Uses:
Medium chain triglycerides (MCTs) are a family of triglycerides, containing predominantly, caprylic (C(8)) and capric (C(10)) fatty acids with lesser amounts of caproic (C(6)) and lauric (C(12)) fatty acids. MCTs are widely used for parenteral nutrition in individuals requiring supplemental nutrition and are being more widely used in foods, drugs and cosmetics.
[Traul KA et al; Food Chem Toxicol 38 (1): 79-98 (2000)] **PEER REVIEWED** PubMed Abstract

Children who suffer from seizures which are not controllable by drugs have apparently been successfully treated with MCT (medium chain triglyceride) diet. The MCT diet is an emulsion containing primarily (81%) octanoic acid, but also contains 15% decanoic acid ... /Medium chain triglyceride/
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.45 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/EXPL THER/ ... The clinical situations requiring total parenteral nutrition (TPN) are associated with metabolic processes mediated by insulin ... Decanoic acid was a potent /insulin/ stimulator in /an isolated perfused mouse islet/ model.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.43 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

/EXPL THER/ The treatment for patients with genetic disorders of mitochondrial long-chain fatty acid beta-oxidation is directed toward providing sufficient sources of energy for normal growth and development, and at the

same time preventing the adverse effects that precipitate or result from metabolic decompensation. Standard of care treatment has focused on preventing the mobilization of lipids that result from fasting and providing medium-chain triglycerides (MCT) in the diet in order to bypass the long-chain metabolic block. MCTs that are currently available as commercial preparations are in the form of even-chain fatty acids that are predominately a mixture of octanoate and decanoate ... The even-numbered medium-chain fatty acids (MCFAs) that are found in MCT preparations can reduce the accumulation of potentially toxic long-chain metabolites of fatty acid oxidation (FAO) ... /Decanoate/
[Jones PM et al; Mol Genet Metab 81(2):96-9 (2004)] **PEER REVIEWED** PubMed Abstract

/VETERINARY ANIMALS/ The most common source of Salmonella infections in humans is food of poultry origin. Salmonella enterica serovar Enteritidis has a particular affinity for the contamination of the egg supply. In this study, the medium-chain fatty acids (MCFA), caproic, caprylic, and capric acid, were evaluated for the control of Salmonella serovar Enteritidis in chickens. All MCFA were growth inhibiting at low concentrations in vitro, with caproic acid being the most potent. Contact of Salmonella serovar Enteritidis with low concentrations of MCFA decreased invasion in the intestinal epithelial cell line T84. By using transcriptional fusions between the promoter of the regulatory gene of the Salmonella pathogenicity island I, hilA, and luxCDABE genes, it was shown that all MCFA decreased the expression of hilA, a key regulator related to the invasive capacity of Salmonella. The addition of caproic acid (3 g/kg of feed) to the feed of chicks led to a significant decrease in the level of colonization of ceca and internal organs by Salmonella serovar Enteritidis at 3 days after infection of 5-day-old chicks. These results suggest that MCFA have a synergistic ability to suppress the expression of the genes required for invasion and to reduce the numbers of bacteria in vivo. Thus, MCFA are potentially useful products for reducing the level of colonization of chicks and could ultimately aid in the reduction of the number of contaminated eggs in the food supply.
[Van Immerseel F et al; Appl Environ Microbiol 70 (6): 3582-7 (2004)] **PEER REVIEWED** PubMed Abstract

/VETERINARY ANIMALS/ Staphylococcus aureus causes a variety of human infections including toxic shock syndrome, osteomyelitis, and mastitis. Mastitis is a common disease in the dairy cow, and S. aureus has been found to be a major infectious organism causing mastitis. The objectives of this research were to determine which FA and esterified forms of FA were inhibitory to growth of S. aureus bacteria. FA as well as their mono-, di-, and triacylglycerol forms were tested for their ability to inhibit a human toxic shock syndrome clinical isolate (MN8) and two S. aureus clinical bovine mastitis isolates (305 and Novel). The seven most potent inhibitors across all strains tested by minimum inhibitory concentration analysis included lauric acid, glycerol monolaurate, capric acid, myristic acid, linoleic acid, cis-9, trans-11 conjugated linoleic acid, and trans-10, cis-12 conjugated linoleic acid. Some of these lipids were chosen for 48-hr growth curve analysis with a bovine mastitis S. aureus isolate (Novel) at doses of 0, 20, 50, and 100 microg/mL except myristic acid, which was tested at 0, 50, 100, and 200 microg/mL. The saturated FA (lauric, capric, myristic) and glycerol monolaurate behaved similarly and reduced overall growth. In contrast, the polyunsaturated FA (linoleic and cis-9, trans-11 conjugated linoleic acid) delayed the time to initiation of exponential growth in a dose-dependent fashion.
[Kelsey JA et al; Lipids 41 (10): 951-61 (2006)] **PEER REVIEWED** PubMed Abstract

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[Morimoto K et al; Drug Dev Ind Pharm 21 (17): 1999-2012 (1995)] **PEER REVIEWED**

Environmental Fate & Exposure:

Environmental Fate/Exposure Summary:
Decanoic acid's production and use in esters for perfumes and fruit flavor, base for wetting agents, intermediates, plasticizer, resins, and as an intermediate for food-grade additives may result in its release to the environment through various waste streams. Decanoic acid has been found in the seeds of American elm (Ulmus americana) and Garcinia mangostana, oil of lime and lemon, and occurs as a glyceride in natural oils. Decanoic acid is a fatty acid and occurs naturally in many essential oils. Fatty acids are widely distributed in nature as components of animal and vegetable fats and are an important part of the normal daily diet of mammals, birds and invertebrates. If released to air, a vapor pressure of 3.66X10-4 mm Hg at 25 deg C indicates decanoic acid will exist solely as a vapor in the atmosphere. Vapor-phase decanoic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 1.4 days. If released to soil, undissociated decanoic acid is expected to have slight mobility based upon an estimated Koc of 4,000 for the free acid. The pKa of decanoic acid is 4.90, indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon the pKa. A 46% of theoretical BOD after 20 days using a sewage inoculum and 42% of theoretical BOD in 1 day using an activated sludge inoculum suggest that biodegradation may be important environmental fate process in soil. If released into water, undissociated decanoic acid is expected to adsorb to suspended solids and sediment based upon the estimated Koc for the free acid. Biodegradation of 100 ppm

decanoic acid using a Japanese cultivation method was 100% in river water and 100% in sea water after 3 days, suggesting that biodegradtion may be an important environmental fate process in water. Volatilization from water surfaces is not expected to be an important fate process based upon the pKa. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to decanoic acid may occur through inhalation and dermal contact with this compound at workplaces where decanoic acid is produced or used. Monitoring data indicate that the general population may be exposed to decanoic acid via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with this compound and other containing decanoic acid. (SRC)
PEER REVIEWED

Probable Routes of Human Exposure:
NIOSH (NOES Survey 1981-1983) has statistically estimated that 7,879 workers (945 of these were female) were potentially exposed to decanoic acid in the US(1). Occupational exposure to decanoic acid may occur through inhalation and dermal contact with this compound at workplaces where decanoic acid is produced or used. Monitoring data indicate that the general population may be exposed to decanoic acid via inhalation of ambient air, ingestion of food and drinking water, and dermal contact with this compound and other containing decanoic acid (SRC).
[(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available at http://www.cdc.gov/noes/ as of Jan 2008.] **PEER REVIEWED**

Body Burden:
Samples of mother's milk were collected from Bayonne, NJ; Jersey City, NJ; Pittsburgh, PA; Baton Rouge, LA; and Charleston, WV and analyzed for volatile and semivolatile organics. Decanoic acid was not detected(1).
[(1) Erickson MD et al; Acquisition and Chemical Analysis of Mother's Milk for Selected Toxic Substances. USEPA-560/13-80-029. Washington, DC: USEPA Off Pestic Toxic Subst pp. 152 (1980)]
PEER REVIEWED

Average Daily Intake:
Fatty acids are an important part of the normal daily diet of mammals, birds and invertebrates.
[USEPA/OPPTS; R.E.D Facts. Soap Salts. Reregistration Eligibility Decisions (REDs) Database. EPA-738-F-92-013. Sept 1992. Available from the Database Query page at http://www.epa.gov/pesticides/reregistration/status.htm as of Sept 8, 2008.] **PEER REVIEWED**

Annual consumption is 18,833.33 lb. Individual consumption is 0.01596 mg/kg/day.
[Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 395] **PEER REVIEWED**

Natural Pollution Sources:
CAPRIC ACID, ISOLATED FROM AMERICAN ELM (ULMUS AMERICANA) SEEDS, WAS IDENTIFIED AS THE ANTIFUNGAL AGENT ACTIVE AGAINST THE DUTCH ELM DISEASE FUNGUS (CERATOCYSTIS ULMI) & SEVERAL OTHER FUNGI.
[DOSKOTCH RW ET AL; PHYTOPATHOLOGY 65(5) 634-5 (1975)] **PEER REVIEWED**

OCTANOIC ACID, DECANOIC ACID, DODECANOIC ACID, TETRADECANOIC ACID, & HEXADECANOIC ACID (11.0-18.7% OF THE TOTAL ACIDS) WERE ISOLATED FROM THE NATURAL SEX PHEROMONES OF MALE MEDITERRANIAN FRUIT FLY (CERATITIS CAPITATA).
[OHINATA K ET AL; J ENVIRON SCI HEALTH PART A A12(3) 67-78 (1977)] **PEER REVIEWED**

NATURAL FOOD OCCURANCES: ANISE, BUTTER ACIDS, OIL OF LIME, OIL OF LEMON.
[CHEMICALS USED IN FOOD PROCESSING; NAS/NRC PUBL 1274 WASHINGTON DC (1965)] **PEER REVIEWED**

CAPRIC ACID (0.9%) WAS FOUND IN THE SEED OIL OF GARCINIA MANGOSTANA.
[DAULATABAD CD, ANKALGI RF; J OIL TECHNOL ASSOC INDIA 10(2) 36-9 (1978)] **PEER REVIEWED**

Occurs as a glyceride in natural oils
[Hawley, G.G. The Condensed Chemical Dictionary. 10th ed. New York: Van Nostrand Reinhold Co., 1981., p. 190] **PEER REVIEWED**

Decanoic acid occurs naturally in various edible and cosmetic oils, eg. coconut oil (up to 9.7%), bay tree oil (37%), and butter fat (2.7%).

[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.45 (2000 CD-ROM edition). Available from, as of January 23, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Decanoic acid was found in fine particulate abrasion products from green leaves at a concn of 183.3 ug/g and from dead leaves at a concn of 133.0 ug/g; samples collected were from trees characteristic of the Los Angeles, CA area (1). Decanoic acid was found as a volatile component of raw earth-almond (Cyperus esculentus L.)(2). The compound is a carboxylic acid that is also known as a fatty acid because fatty acids were first isolated by the hydrolysis of naturally occurring fats(3). Fatty acids are widely distributed in nature as components of animal and vegetable fats(4) including lipids such as oils and fats, waxes, sterol esters and other minor compounds(3).
[(1) Rogge WF et al; Environ Sci Technol 27: 2700-11 (1993) (2) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997) (3) Gutsche CD, Pasto DJ; Fundamentals of Organic Chemistry. Englewood Cliffs, NJ: Prentice-Hall p. 369 (1975) (4) Anneken DJ et al; Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (2008). NY, NY: John Wiley & Sons; Fatty Acids. Online Posting Date: Dec 15, 2006.] **PEER REVIEWED**

Artificial Pollution Sources:
Decanoic acid's production and use in esters for perfumes and fruit flavor, base for wetting agents, intermediates, plasticizer, resins and as an intermediate for food-grade additives(1) may result in its release to the environment through various waste streams(SRC).
[(1) Lewis RJ; Hawley's Condensed Chemical Dictionary. 14th Ed. NY, NY: John Wiley & Sons, Inc. p. 203 (2001)] **PEER REVIEWED**

Environmental Fate:
TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 4,000 for the free acid(SRC), determined from a log Kow of 4.09(2) and a regression-derived equation(3), indicates that undissociated decanoic acid is expected to have slight mobility in soil(SRC). The pKa of decanoic acid is 4.90(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5). Volatilization of decanoic acid from moist soil surfaces is not expected to be an important fate process based upon the pKa(SRC). Decanoic acid is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 3.66X10-4 mm Hg (6). A 46% of theoretical BOD after 20 days in the presence of sewage inoculum(7) and 42% of theoretical BOD in 1 day using an activated sludge inoculum(8) suggest that biodegradation may be important environmental fate process in soil.
[(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 81 (1995) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (4) Barratt MD; Toxicol In Vitro 10:85-94 (1996) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (6) Baccanari DP et al; Trans Faraday Soc 64: 1201-5 (1968) (7) Gaffney PE, Heukelekian H; J Water Pollut Control Fed 33: 1169-83 (1961) (8) Malaney GW, Gerhold RM; pp. 249-257 in Proc 17th Ind Waste Conf, Purdue Univ, Ext Ser 112 (1962)] **PEER REVIEWED**

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 4,000 for the free acid(SRC), determined from a log Kow of 4.09(2) and a regression-derived equation(3), indicates that undissociated decanoic acid is expected to adsorb to suspended solids and sediment(SRC). A pKa of 4.90(4) indicates decanoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore volatilization from water surfaces is not expected to be an important fate process(5). According to a classification scheme(6), an estimated BCF of 3(SRC), from its log Kow(2) and a regression-derived equation(7), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Biodegradation of 100 ppm decanoic acid using a Japanese cultivation method was 100% in river water and 100% in sea water after 3 days(8), suggesting that biodegradtion may be an important environmental fate process in water(SRC).
[(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 81 (1995) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990) (4) Barratt MD; Toxicol In Vitro 10:85-94 (1996) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds, Boca Raton, FL: Lewis Publ (2000) (6) Franke C et al; Chemosphere 29: 1501-14 (1994) (7) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (8) Kondo M et al; Eisei Kagaku 34: 188-95 (1988)] **PEER REVIEWED**

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), decanoic acid, which has a vapor pressure of 3.66X10-4 mm Hg at 25 deg C(2), is expected to

exist solely as a vapor in the ambient atmosphere. Vapor-phase decanoic acid is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 1.4 days(SRC), calculated from its rate constant of 1.1X10-11 cu cm/molecule-sec at 25 deg C(SRC) that was derived using a structure estimation method(3).
[(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Baccanari DP et al; Trans Faraday Soc 64: 1201-5 (1968) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)] **PEER REVIEWED**

Environmental Biodegradation:
AEROBIC: The 5 day BOD of decanoic acid, concn 100 ppm, was determined to be 8.52 mmol/mmol decanoic acid using acclimated mixed microbial cultures in a mineral salt medium(1). Decanoic acid, present at 10,000 ppm, reached 45 to 53% and 46 to 54% of its theoretical BOD in 5 and 20 days, respectively, using a sewage inoculum (2). Decanoic acid, present at 10,000 ppm, reached 13, 45, and 46% of its theoretical BOD in 5, 10, and 20 days, respectively, using a sewage inoculum(3). In a similar study, decanoic acid, present at 10,000 ppm, reached 49, 53, and 54% of its theoretical BOD in 5, 10, and 20 days, respectively, using an acclimated sewage inoculum(3). Decanoic acid, present at unknown concn, reached 9% of its theoretical BOD in 5 days using a sewage inoculum (4). Using the Warburg test method, decanoic acid, present at 500 ppm, reached 29 to 42% of its theoretical BOD in 1 day, using an activated sludge inoculum with a microbial population of 2,500 mg/L corrected for endogenous respiration(5). Biodegradation of 100 ppm decanoic acid using the cultivation method was 100% in river water and 100% in sea water after 3 days(6). The theoretical oxygen demand for 500 mg/L decanoic acid was determined to be 10.9%, 18.9%, and 23.4% after 6, 12, and 24 hours of exposure to activated sludge solids at 2,500 mg/L in the Warburg respirometer(7). An aerobic biodegradation screening study of decanoic acid, based on BOD measurements, using a sewage inoculum and an unknown decanoic acid concn, indicated 23% of its theoretical BOD over a period of 20 days(8). The biodegradation of 100 mg/L decanoic acid by non-acclimated activated sludge over an unspecified time period was determined to have 100% total organic carbon removal(9).
[(1) Babeu L, Vaishnav DD; J Indust Microbiol 2: 107-15 (1987) (2) Gaffney PE, Heukelekian H; J Water Pollut Control Fed 30: 673-79 (1958) (3) Gaffney PE, Heukelekian H; J Water Pollut Control Fed 33: 1169-83 (1961) (4) Dore M et al; Trib Cebedeau 28: 3-11 (1975) (5) Malaney GW, Gerhold RM; pp. 249-257 in Proc 17th Ind Waste Conf, Purdue Univ, Ext Ser 112 (1962) (6) Kondo M et al; Eisei Kagaku 34: 188-95 (1988) (7) Malaney GW, Gerhold RM; J Water Poll Control Fed 41: R18-R33 (1969) (8) Nieme GJ et al; Environ Toxicol Chem 6: 515-27 (1987) (9) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 12: 85-91 (1982)] **PEER REVIEWED**

Environmental Abiotic Degradation:
The rate constant for the vapor-phase reaction of decanoic acid with photochemically-produced hydroxyl radicals has been estimated as 1.1X10-11 cu cm/molecule-sec at 25 deg C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 1.4 days at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). Decanoic acid is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions(2). Decanoic acid was present at 1.5 mg/L in the influent to a continuous retort water treatment cell; after 1, 3 and 5 weeks decanoic acid was not detected, and after 7 weeks decanoic acid was found at 108.6 mg/L, indicating adsorption followed by desorption(3).
[(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990) (3) Syamsiah S et al; Fuel 72: 855-61 (1993)] **PEER REVIEWED**

Environmental Bioconcentration:
An estimated BCF of 3 was calculated in fish for decanoic acid(SRC), using a log Kow of 4.09(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).
[(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 81 (1995) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)] **PEER REVIEWED**

Soil Adsorption/Mobility:
The Koc of undissociated decanoic acid is estimated as 4,000 forthe free acid Kow of 4.09(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that undissociated decanoic acid is expected to have slight mobility in soil. The pKa of decanoic acid is 4.90(4), indicating that this compound will exist almost entirely in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).
[(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref

Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 81 (1995) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (3) Swann RL et al; Res Rev 85: 17-28 (1983) (4) Barratt MD; Toxicol In Vitro 10:85-94 (1996) (5) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)] **PEER REVIEWED**

Volatilization from Water/Soil:
A pKa of 4.90(1) indicates decanoic acid will exist almost entirely in the anion form at pH values of 5 to 9 and therefore volatilization from water surfaces and moist soil is not expected to be an important fate process(2). Decanoic acid is not expected to volatilize from dry soil surfaces(SRC) based upon a vapor pressure of 3.66X10-4 mm Hg(3).
[(1) Barratt MD; Toxicol In Vitro 10:85-94 (1996) (2) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (3) Baccanari DP et al; Trans Faraday Soc 64: 1201-5 (1968)] **PEER REVIEWED**

Environmental Water Concentrations:
GROUNDWATER: Groundwater samples taken from wells in the Besos basin, Northeast Spain were found to contain decanoic acid concentrations ranging from 42 to 75 ng/L(1).
[(1) Guardiola J et al; Water Supply 7: 11-16 (1989)] **PEER REVIEWED**

DRINKING WATER: Decanoic acid was identified in the initial survey of raw and treated water taken at waterworks treating lowland river water in the UK between March and December 1976(1). In the survey of treated water, decanoic acid was identified in 3 of 14 samples taken between Feb and June 1979 after new treatment procedures were implemented(1). Decanoic acid has been quantitatively detected, concn not reported, in drinking water samples collected from Poplarville, MS on March 2, 1979; Cincinnati, OH on October 17, 1978; Cincinnati, OH on January 14, 1980; New Orleans, LA on January 14, 1976; Miami, FL on February 3, 1976; Philadelphia, PA on February 10, 1976; Ottumwa, IA on September 10, 1976 and Seattle, WA on November 5, 1976(2). Decanoic acid has been identified as an organic disinfection byproduct (DBP) at a pilot plant in Evansville, IN, concn not reported (3). Decanoic acid was identified as an ozone disinfection by-product in drinking water samples from a pilot plant in Jefferson Parish, LA which uses Mississippi River was as the raw water source; samples were collected following 4 rounds of ozonation treatment performed in January, 1994, August 1994, May 1995, and September 1996(4).
[(1) Fielding M et al; Organic Micropollutants in Drinking Water; TR-159. Medmenham: Eng Water Res Cent (1981) (2) Lucas SV; GC/MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates; Vol 1: Analysis Results for 17 Drinking Water, 16 Advanced Waste Treatment, ad 3 Process Blank Concentrates. USEPA-600/1-84-020A (NTIS PB85-128221) Columbus, OH: Batelle Columbus Labs, Health Eff Res Lab (1984) (3) Richardson SD et al; Environ Sci Technol 28: 592-99 (1994) (4) Richardson SD et al; Environ Sci Technol 33: 3368-77 (1999)] **PEER REVIEWED**

RAIN/SNOW: Decanoic acid has been identified in rain/snow: aqueous (wet-only) from rural Hubbard Brook, NH and semi-rural Ithaca, NY; samples collected between June 1976 and May 1977 were determined to have an average decanoic acid concn of < 0.1 umol/75 cm precipitate(1). Decanoic acid was identified at 5 of 10 snow sample sites in Russia and Finland; 0.06 ug/kg at Nellim (Lapland, Finland), 0.07 ug/kg at Muonio (Lapland, Finland), 0.36 ug/kg at Levi (Lapland, Finland), 0.03 ug/kg at Butovo (Moscow, Russia) and 0.22 ug/kg at Moscow State University (Moscow, Russia)(2).
[(1) Mazurek MA, Simoneit BRT; CRC Critical Reviews in Environmental Control 16: 1-140 (1986) (2) Poliakova OV et al; Toxicol Environ Chem 75: 181-94 (2000)] **PEER REVIEWED**

Effluent Concentrations:
An average decanoic acid concn of 1,788 ng/uL was identified in an industrial wastewater survey in which samples collected between Nov 1, 1979 to Nov 1, 1981 were analyzed for organic pollutants other than Priority Pollutants (1). Oil shale retort water from Rundle, Australia was found to contain decanoic acid at a concn of 45 mg/L(2). Decanoic acid was identified in vapor at a concn of 10 ng/cu m and on particles with a concn of 20 ng/g emitted during combustion of coal at Ames power plant in Iowa(3). Two oil-shale retort water samples produced from Jan to May 1979 at the Occidental Oil Shale, Inc. facility at Logan Wash, CO were reported to have an average decanoic acid concn of 31 mg/L(4). 63 Effluent water samples from industrial sites in Ohio, West Virginia, Pennsylvania, New Jersey, New York, Louisiana, Kentucky, Delaware, and Texas were collected and analyzed for decanoic acid. Site 26 reported a decanoic acid concn between 10 to 100 ug/L. Site 31 reported a decanoic acid concn ranging from < 10 to 100 ug/L(5). Decanoic acid was identified at a concn of 3 ppb in process water effluent samples (from in situ coal gasification) from Gilette, WY and 123 ppb from boiler blowdown water effluent samples (from in situ oil shale processing) from DeBeque, CO(6). Decanoic acid was identified in Iona Island Sewage Treatment Plant(British Columbia, Canada) sewage and sludge effluent, concns up to 30 ug/L(7). Secondary effluents from ten municipal and industrial wastewater treatment plants discharging into Illinois rivers were

sampled; decanoic acid was identified in effluents from St. Charles Public Owned Treatment Works (POTW), Addison POTW, and Decatur POTW, concn unknown(8). Decanoic acid was identified in trench leachates from Maxey Flats (Morehead), KY disposal site, concn unknown and West Valley, NY disposal site, concn ranging from 0.87 to 2.6 mg/L(9).
[(1) Bursey JT, Pellizzari ED; Analysis of Industrial Wastewater for Organic Pollutants in Consent Degree Survey Contract No 68-03-2867 Athens, GA: USEPA Environ Res Lab pp 167 (1982) (2) Dobson KR et al; Water Res 19: 849-56 (1985) (3) Junk GA et al; in ACS Symposium Ser 319 (Fossil Fuels Util): 109-319 (1986) (4) Leenheer JA et al; Environ Sci Technol 16: 714-23 (1982) (5) Perry DL et al; Identification of Organic Compounds in Industrial Effluent Discharges. USEPA-560/6-78-009 NTIS PB-2919000 Columbus, OH: Batelle Columbus Labs (1978) (6) Pellizari ED et al; in ASTM Spec Tech Publ, STP 686: 256-74 (1979) (7) Rogers IH et al; Water Poll Res J Canada 21: 187-204 (1986) (8) Ellis DD et al; Arch Environ Contam Toxicol 11: 373-82 (1982) (9) Francis AJ et al; Nuclear Technology 50: 158-63 (1980)] **PEER REVIEWED**

Fine aerosol particulate-phase emission rates for decanoic acid from noncatalyst automobiles, catalyst automobiles, and heavy-duty diesel trucks were determined to be 3.2, 72.7, and 77.4 ug/km, respectively(1). Decanoic acid was identified in tire wear particles, brake lining particles, and road dust particles at concns of 37.8, 18.4, and 55.4 ug/g of particle sample, respectively(2). Decanoic acid was emitted from medium duty diesel trucks at 72.9 ug/km(3). Decanoic acid was measured in the gas-phase emissions of gasoline powered motor vehicles at a rate of 9.3 ug/km and 54.7 ug/km for catalyst equipped engines and non-catalyst equipped engines, respectively (4).
[(1) Rogge WF et al; Environ Sci Technol 27: 636-51 (1993) (2) Rogge WF et al; Environ Sci Technol 27: 1892-1904 (1993) (3) Schauer JJ et al; Environ Sci Technol 33: 1578-87 (1999) (4) Schauer JJ et al; Environ Sci Technol 36: 1169-80 (2002)] **PEER REVIEWED**

Decanoic acid was found in candle smoke from paraffin and beeswax at 0.16 and 0.32 mg/g of organic compounds (1). Decanoic acid was found in wood smoke from red maple, red oak, paper birch, white pine, hemlock, and balsam fir(2). Decanoic acid was detected in wood smoke from pine, oak and synthetic logs at 0.095, 0.39 and 0.70 mg/kg of wood burnt(3). Decanoic acid was found in the fine aerosols from boilers burning number 2 distillate fuel oil at a rate of 337.3 pg/kJ (burning at 58% capacity with 6.5% excess oxygen in stack gases) and a rate of 58.4 pg/kJ (burning at 54% capacity with 7.1% excess oxygen in stack gases)(4). Fine particle emission rates for decanoic acid from a natural gas-fired water heater and a natural gas-fired space heater were determined. A HEPA-filtered dilution air sample emission rate for decanoic acid was determined to be 2.9 pg/kJ; the emission rate for decanoic acid through the first filter was determined to be 119.5 pg/kJ; the emission rate for decanoic acid through the backup filter was determined to be 131.3 pg/kJ(5). Decanoic acid was found at 2,043.0 ug/g from heated roofing tar pot fumes(6). Decanoic acid was found in gas and particulate matter effluents from commercial-scale meat charbroiling operations at 8,890 and 2,220 ug/kg meat cooked, respectively(7).
[(1) Fine PM et al; Environ Sci Technol 33: 2352-62 (1999) (2) Fine PM et al; Environ Sci Technol 35: 2665-75 (2001) (3) Rogge WF et al; Environ Sci Technol 32: 13-22 (1998) (4) Rogge WF et al; Environ Sci Technol 31: 2731-7 (1997) (5) Rogge WF et al; Environ Sci Technol 27: 2736-44 (1993) (6) Rogge WF et al; Environ Sci Technol 31: 2726-30 (1997) (7) Schauer JJ et al; Environ Sci Technol 33: 1566-77 (1999)] **PEER REVIEWED**

Sediment/Soil Concentrations:
SEDIMENT: Sediment samples collected on September 28, 1990 from Dokai Bay in north Kyushu, Japan were found to contain decanoic acid at unknown concentrations(1). Decanoic acid was identified in sediment samples taken Sept 1995 at the mouth of 3 rivers and in 1 port in Niigata, Japan(2).
[(1) Terashi A et al; Bull Environ Contam Toxicol 50: 348-55 (1993) (2) Kawata K et al; Bull Environ Contam Toxicol 65: 660-7 (2000)] **PEER REVIEWED**

Atmospheric Concentrations:
URBAN/SUBURBAN: Sampling of particulate matter and gaseous pollutants was conducted for three weeks between October 7, 1976 and October 29, 1976 in Belgium; decanoic acid was identified in the gas phase of the urban air samples, concn unknown(1). Aerosol samples were collected systematically throughout a complete annual cycle (1982) at four urban sites in southern California. Ambient annual concns of decanoic acid ranged from 1.3 to 3.1 ng/cu-m(2). Decanoic acid had an average concentration of 3.2 ng/cu m in 4 urban sites from southern CA from samples taken Sept 8-9, 1993(3). Decanoic acid was found at 0.001-0.004, 0.001-0.002, 0.003-0.004, and 0.004-0.011 ppbv at UCLA campus, Newberry Park, Monterey Park, and La Habra, CA in Oct 1984(4). Decanoic acid was detected at 0.04, 0.06, 0.05 and 0.07 ug/cu m in Long Beach, Los Angeles, Azusa and Claremont, CA, respectively, Sept 8-9, 1993(5). Atmospheric samples taken Dec 26-28, 1995 and Jan 4-6, 1996 in Fresno, CA had 0.711 and 0.211ng/cu m and samples taken in Bakersfield had 0.164 and 0.244 ng/cu m of decanoic acid, respectively(6).
[(1) Cautreels W, VanCauwenberghe K; Atmos Environ 12: 1133-41 (1978) (2) Rogge WF et al; Atmos Environ 27A: 1309-30 (1993) (3) Fraser MP et al; Environ Sci Technol 37: 446-53 (2003) (4)

Kawamura K et al; Atmos Environ 34: 4175-91 (2000) (5) Nolte CG et al; Environ Sci Technol 33: 540-5 (1999) (6) Schauer JJ, Cass GR; Environ Sci Technol 34: 1821-32 (2000)] **PEER REVIEWED**

RURAL/REMOTE: Decanoic acid was found on aerosols obtained over the southern North Atlantic Ocean with a mean concn of 4.9 ng/cu m(1). Analysis of the atmosphere in the Eggegebirge forest in North Rhine-Westflia, western Germany was found to contain decanoic acid, concns unknown(2). Aerosol samples were collected from a tower on Enewetak Atoll 1, Marshall Islands, a tower on the RV Moana Wave in the North Pacific Ocean and from American Somoa; decanoic acid concns were determined to be 0.11, 0.025, and 0.49 to 3.7 ng/cu m, respectively (3). Decanoic acid was found in 20% of samples taken near a lighthouse in Fajardo and was also detected in the open ocean off the south coast of Puerto Rico(4). Decanoic acid was not detected on San Nicolas Island, CA, Sept 8-9, 1993(5). Atmospheric samples taken Dec 26-28, 1995 and Jan 4-6, 1996 in Kern Wildlife Refuge, CA had 0.098 and 0.105 ng/cu m of decanoic acid(6).
[(1) Duce RA et al; Rev Geophysics Space Physics 21: 921-52 (1983) (2) Helmig D et al; Chemosphere 19: 1399-1412 (1989) (3) Kawamura K, Gagosian RB; Nature 325: 330-32 (1987) (4) Mayol-Bracero OL et al; Atmos Environ 35: 1735-45 (2001) (5) Nolte CG et al; Environ Sci Technol 33: 540-5 (1999) (6) Schauer JJ, Cass GR; Environ Sci Technol 34: 1821-32 (2000)] **PEER REVIEWED**

Food Survey Values:
Flavoring constituents of cassava (Manihot esculenta) from the Dominican Republic, gari from Nigeria, and farine from the Caribbean (St. Lucia) were analyzed. Decanoic acid was identified in gari, amounts unknown(1). The decanoic acid content in milk fat from cows ranges from 1.19 to 2.01 percent of total fatty acid content(2). Decanoic acid was identified in raw beef using supercritical carbon dioxide extraction; 0.10 percent of the noncondensable volatile fraction area was identified as decanoic acid(3). Decanoic acid was identified as a volatile constituent of cooked strawberry jam at a concn of 6.1 mg/kg(4). Decanoic acid has been identified in mutton and beef volatiles, concn unknown(5). The fine aerosol emission rate for decanoic acid from a frying hamburger (extralean/regular), from a charbroiled hamburger (extralean), and from a charbroiled hamburger (regular) was determined to be 3.5, 16.3, and 25.0 mg/kg, respectively(6). Decanoic acid was found as a volatile component of raw and roasted earth-almond (Cyperus esculentus L.)(7). Decanoic acid occurs as a component (along with caprylic acid and behenic acid) of caprenin, a triglyceride used as a low calorie cocoa butter substitute(8).
[(1) Dougan J et al; J Sci Food Agric 34: 874-84 (1983) (2) Hall CW; Kirk-Othmer Encycl Chem Tech. 4th ed. NY,NY: John Wiley and Sons 16: 705 (1995) (3) King MF et al; J Agric Food Chem 41: 1974-81 (1993) (4) Lesschaeve I et al; J Food Science 56: 1393-98 (1991) (5) Shahidi F et al; CRC Crit Rev Food Sci Nature 24: 141-243 (1986) (6) Rogge WF et al; Environ Sci Technol 25: 1112-25 (1991) (7) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997) (8) Friedman LJ et al; Kirk-Othmer Encycl Chem Tech. 4th ed. NY,NY: John Wiley and Sons 11: 815 (1994)] **PEER REVIEWED**

Decanoic acid was found in gas and particulate matter effluents from commercial-scale meat charbroiling operations at 8,890 and 2,220 ug/kg meat cooked, respectively(1).
[(1) Schauer JJ et al; Environ Sci Technol 33: 1566-77 (1999)] **PEER REVIEWED**

Plant Concentrations:
Decanoic acid was found in fine particulate abrasion products from green leaves at a concn of 183.3 ug/g and from dead leaves at a concn of 133.0 ug/g; samples collected were from trees characteristic of the Los Angeles, CA area (1). Decanoic acid was found as a volatile component of raw earth-almond (Cyperus esculentus L.)(2).
[(1) Rogge WF et al; Environ Sci Technol 27: 2700-11 (1993) (2) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997)] **PEER REVIEWED**

Milk Concentrations:
ENVIRONMENTAL: The decanoic acid content in milk fat from cows ranges from 1.19 to 2.01 percent of total fatty acid content(1). Decanoic acid was not detected in samples of mother's milk that were collected from Bayonne, NJ; Jersey City; NJ, Pittsburgh, PA; Baton Rouge, LA; and Charleston, WV and analyzed for volatile and semivolatile organics(2).
[(1) Hall CW; Kirk-Othmer Encycl Chem Tech. 4th ed. NY,NY: John Wiley and Sons 16: 705 (1995) (2) Erickson MD et al; Acquisition and Chemical Analysis of Mother's Milk for Selected Toxic Substances. USEPA-560/13-80-029. Washington, DC: USEPA Off Pestic Toxic Subst pp. 152 (1980)] **PEER REVIEWED**

Other Environmental Concentrations:
Decanoic acid was detected not quantified in settled household dust samples collected in January-February from 12 houses in urban areas in central Finland(1). Decanoic acid was not detected in unburned paraffin and beeswax(2).
[(1) Hirvonen A et al; Indoor Air 4: 255-64 (1994) (2) Fine PM et al; Environ Sci Technol 33:

2352-62 (1999)] **PEER REVIEWED**

Environmental Standards & Regulations:

FIFRA Requirements:
Residues of the following chemical substances are exempted from the requirement of a tolerance when used in accordance with good manufacturing practice as ingredients in an antimicrobial pesticide formulation, provided that the substance is applied on a semi-permanent or permanent food-contact surface (other than being applied on food packaging) with adequate draining before contact with food. ... (b) The following chemical substances when used as ingredients in an antimicrobial pesticide formulation may be applied to: Dairy processing equipment, and food-processing equipment and utensils. Decanoic acid is included on this list. Limit: when ready for use, the end-use concentration is not to exceed 90 ppm.
[40 CFR 180.940(b) (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.gpoaccess.gov/ecfr **PEER REVIEWED**

An exemption from the requirement of a tolerance is established for residues of decanoic acid in or on all raw agricultural commodities and in processed commodities, when such residues result from the use of decanoic acid as an antimicrobial treatment in solutions containing a diluted end-use concentration of decanoic acid (up to 170 ppm per application) on food contact surfaces such as equipment, pipelines, tanks, vats, fillers, evaporators, pasteurizers and aseptic equipment in restaurants, food service operations, dairies, breweries, wineries, beverage and food processing plants
[40 CFR 180.1225 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.gpoaccess.gov/ecfr **PEER REVIEWED**

FDA Requirements:
Capric acid is a food additive permitted for direct addition to food for human consumption, as long as 1) the quantity of the substance added to food does not exceed the amount reasonably required to accomplish its intended physical, nutritive, or other technical effect in food, and 2) any substance intended for use in or on food is of appropriate food grade and is prepared and handled as a food ingredient.
[21 CFR 172.860 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.gpoaccess.gov/ecfr **PEER REVIEWED**

Allowable Tolerances:
Residues of the following chemical substances are exempted from the requirement of a tolerance when used in accordance with good manufacturing practice as ingredients in an antimicrobial pesticide formulation, provided that the substance is applied on a semi-permanent or permanent food-contact surface (other than being applied on food packaging) with adequate draining before contact with food. ... (b) The following chemical substances when used as ingredients in an antimicrobial pesticide formulation may be applied to: Dairy processing equipment, and food-processing equipment and utensils. Decanoic acid is included on this list. Limit: when ready for use, the end-use concentration is not t exceed 90 ppm.
[40 CFR 180.940(b) (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.gpoaccess.gov/ecfr **PEER REVIEWED**

An exemption from the requirement of a tolerance is established for residues of decanoic acid in or on all raw agricultural commodities and in processed commodities, when such residues result from the use of decanoic acid as an antimicrobial treatment in solutions containing a diluted end-use concentration of decanoic acid (up to 170 ppm per application) on food contact surfaces such as equipment, pipelines, tanks, vats, fillers, evaporators, pasteurizers and aseptic equipment in restaurants, food service operations, dairies, breweries, wineries, beverage and food processing plants
[40 CFR 180.1225 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of February 1, 2008: http://www.gpoaccess.gov/ecfr **PEER REVIEWED**

Chemical/Physical Properties:

Molecular Formula:
C10-H20-O2
PEER REVIEWED

Molecular Weight:
172.27
[Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-134] **PEER REVIEWED**

Color/Form:
Crystalline solid
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 285] **PEER REVIEWED**

White crystals
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 203] **PEER REVIEWED**

Needles
[Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-124] **PEER REVIEWED**

White crystals or needles
[Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 10th ed. Volumes 1-3 New York, NY: John Wiley & Sons Inc., 1999., p. V2: 1079] **PEER REVIEWED**

Pale yellow solid
[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

Odor:
Rancid odor
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 285] **PEER REVIEWED**

Unpleasant odor
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 203] **PEER REVIEWED**

Boiling Point:
268.7 deg C
[Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-134] **PEER REVIEWED**

Melting Point:
31.5 deg C
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 203] **PEER REVIEWED**

Density/Specific Gravity:
0.890 at 40 deg C/4 deg C
[Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V3: 2427] **PEER REVIEWED**

Dissociation Constants:
pKa = 4.90
[Barratt MD; Toxicol In Vitro 10: 85-94 (1996)] **PEER REVIEWED**

Heat of Combustion:
-6,108.7 kJ/mol
[Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5: 147-168 (1993)] **PEER REVIEWED**

Octanol/Water Partition Coefficient:
log Kow = 4.09
[Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 81] **PEER REVIEWED**

Solubilities:
Practically insol in water (0.015 g/100 g at 20 deg C); sol in ethanol; ether; chloroform; benzene; carbon disulfide; dilute nitric acid
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 285] **PEER REVIEWED**

Very soluble in acetone, benzene, ethyl ether, ethanol
[Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-134] **PEER REVIEWED**

Soluble in most organic solvents and dilute nitric acid
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 203] **PEER REVIEWED**

In water solubility, 61.8 mg/L at 25 deg C
[Yalkowsky SH, Dannenfelser RM; The AQUASOL dATAbASE of Aqueous Solubility. Fifth ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)] **PEER REVIEWED**

Spectral Properties:
Index of refractoin: 1.4288 at 40 deg C/D
[Lide, D.R. CRC Handbook of Chemistry and Physics 86TH Edition 2005-2006. CRC Press, Taylor & Francis, Boca Raton, FL 2005, p. 3-134] **PEER REVIEWED**

SADTLER REFERENCE NUMBER: 2705 (IR, PRISM)
[Weast, R.C. (ed.). Handbook of Chemistry and Physics. 57th ed. Cleveland: CRC Press Inc., 1976., p. C-271] **PEER REVIEWED**

IR: 215 (Coblentz Society Spectral Collection)
[Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V3: 2427] **PEER REVIEWED**

NMR: 6723 (Sadtler Research Laboratories Spectral Collection)
[Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V3: 2427] **PEER REVIEWED**

MASS: 36479 (NIST/EPA/MSDC Mass Spectral database, 1990 version)
[Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V3: 2427] **PEER REVIEWED**

Surface Tension:
25.0 mN/m (= dyn/cm) at 70 deg C
[Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5: 147-168 (1993)] **PEER REVIEWED**

Vapor Pressure:
3.66X10-4 mm Hg at 25 deg C
[Baccanari DP et al; Trans Faraday Soc 64: 1201-5 (1968)] **PEER REVIEWED**

Viscosity:
4.30 mPa.sec (= cP) at 50 deg C

[Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V5: 147-168 (1993)] **PEER REVIEWED**

Other Chemical/Physical Properties:
Precipitates unchanged from dil nitric acid (density 1.14) by addition of water
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 285] **PEER REVIEWED**

Acid value: 320 to 330 mg KOH/g
[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

Density/Specfific gravity: 0.88 kg/l at 4 deg C
[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

Henry's Law constant = 1.34X10-6 atm-cu m/mole at 25 deg C (est)
[SRC; The Physical Properties Database (PHYSPROP). Syracuse, NY: Syracuse Res Corp. Available from, as of Dec 18, 2007: http://www.syrres.com/esc/physprop.htm **PEER REVIEWED**

Hydroxyl radical reaction rate constant = 1.12X10-11 cu cm/molec-sec at 25 deg C (est)
[US EPA; Estimation Program Interface (EPI) Suite. Ver.3.12. Nov 30, 2004. Available from, as of Dec 18, 2007: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm **PEER REVIEWED**

Chemical Safety & Handling:

Odor Threshold:
Aroma threshold values: Detection: 2.2 to 102 ppm.
[Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 395] **PEER REVIEWED**

Skin, Eye and Respiratory Irritations:
n-Decanoic acid was irritant to the skin of humans ... No skin sensitization was induced in volunteers treated with a dilute solution.
[British Industrial Biological Research Association (BIBRA) Working Group; BIBRA Toxicology International 6: (1996)] **PEER REVIEWED**

Fire Potential:
Combustible
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

Hazardous Decomposition:
When heated to decomposition it emits acrid smoke and irritating fumes.
[Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 1075] **PEER REVIEWED**

Preventive Measures:
Wear the items of protective clothing the label requires: for example, non-absorbent gloves (not leather or fabric), rubber footwear (not canvas or leather), a hat, goggles, or a dust-mist filter. If no specific clothing is listed, gloves, long-sleeved shirts and long pants, and closed shoes are recommended. You can buy protective clothing and equipment at hardware stores or building supply stores. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.19 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Indoor Applications. If the label directions permit, leave all windows open and fans operating after the application is completed. If the pesticide product is only effective in an unventilated (sealed) room or house, do not stay there. Put all pets outdoors, and take yourself any your family away from treated areas for at least the length of time prescribed on the label. Apply most surface sprays only to limited areas such as cracks; don't treat entire

floors, walls, or ceilings. Don't let pesticides get on any surfaces that are used for food preparation. Wash any surfaces that may have pesticide residue before placing food on them. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.20 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Indoor Applications. When using total release foggers to control pests, use no more than the amount needed and to keep foggers away from ignition sources (ovens, stoves, air conditioners, space heaters, and water heaters, for example). Foggers should not be used in small, enclosed places such as closets and cabinets or under tables and counters. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.21 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Outdoor Applications. Never apply pesticides outdoors on a windy day (winds higher than 10 mph). Position yourself so that a light breeze does not blow pesticide spray or dust into your face. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.21 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Storage Conditions:
Safe Storage of Pesticides. Always store pesticides in their original containers, complete with labels that list ingredients, directions for use, and first aid steps in case of accidental poisoning. Never store pesticides in cabinets with or near food, animal feed, or medical supplies. Do not store pesticides in places where flooding is possible or in places where they might spill or leak into wells, drains, ground water, or surface water. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.23 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Cleanup Methods:
If a spill occurs, clean it up promptly. Don't wash it away. Instead, sprinkle the spill with sawdust, vermiculite, or kitty litter. Sweep it into a plastic garbage bag, and dispose of it as directed on the pesticide product label./Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.20 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

After Applying a Pesticide, Indoors or Outdoors. To remove pesticide residues, use a bucket to rinse tools or equipment three times, including any containers or utensils that you used when mixing the pesticide. Then pour the rinsewater into the pesticide sprayer and reuse the solution by applying it according to the pesticide product label directions. After applying any pesticide wash your hands and any other parts of your body that may have come in contact with the pesticide..To prevent tracking pesticides inside, remove or rinse your boots or shoes before entering your home. Wash any clothes that have been exposed to a lot of pesticide separately from your regular wash. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.22 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Disposal Methods:
SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.
PEER REVIEWED

Safe Disposal of Pesticides. The best way to dispose of small amounts of excess pesticides is to use them - apply them - according to the directions on the label. If you cannot use them, ask your neighbors whether they have a similar pest control problem and can use them. If all of the remaining pesticide cannot be properly used, check with your local solid waste management authority, environmental agency, or health department to find out whether your community has a household hazardous waste collection program or a similar program for getting rid of unwanted, leftover pesticides. These authorities can also inform you of any local requirements for pesticide waste disposal. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.24 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Safe Disposal of Pesticides. An empty pesticide container can be as hazardous as a full one because of residues left inside. Never reuse such a container. When empty, a pesticide container should be rinsed carefully three times and the rinsewater thoroughly drained back onto the sprayer or the container previously used to mix the pesticide. Use

the rinsewater as a pesticide, following label directions. Replace the cap or closure securely. Dispose of the container according to label instructions. Do not puncture or burn a pressurized container like an aerosol - it could explode. Do cut or puncture other empty pesticide containers made of metal or plastic to prevent someone from reusing them. Wrap the empty container and put it in the trash after you have rinsed it. /Residential uses/
[USEPA/Prevention, Pesticides, and Toxic Substances; Citizen's Guide to Pest Control and Pesticide Safety p.25 (September 1995) EPA 730-K-95-001] **PEER REVIEWED**

Occupational Exposure Standards:

Manufacturing/Use Information:

Major Uses:
For Capric acid (USEPA/OPP Pesticide Code: 128955) ACTIVE products with label matches. /SRP: Registered for use in the U.S. but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently approved uses./
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

Esters for perfumes and fruit flavor, base for wetting agents; intermediates; plasticizer; resins; intermediate for food-grade additives
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

Chemical intermediate for the synthesis of capryl imidazoline, ethyl caprate
[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

Use resulting in inclusion into or onto matrix ... paints, lacquers and varnishes industry ... solvents ...
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.4 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

Reported uses (ppm):
Reported uses (ppm): (Flavor and Extract Manufacturers' Association)

Food Category	Usual	Max.
Baked goods	9.56	12.39
Cheese	10.70	10.80
Chewing gum	0.00	0.01
Fats, oils	4.47	8.97
Frozen dairy	1.61	7.45
Gelatins, puddings	0.49	2.06
Gravies	0.30	0.60
Imitation dairy	7.00	14.00
Meat products	1.89	2.00
Nonalcoholic beverages	0.98	1.57
Snack foods	2.00	2.00
Soft candy	1.90	6.13

[Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 395] **PEER REVIEWED**

Manufacturers:

Penta Manufacturing Co., 50 Okner Pkwy., Livingston, NJ 07039-1604, (973) 740-2300; Production site: Fairfield, NJ 07004
[SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 602] **PEER REVIEWED**

The Procter & Gamble Company, 1 or 2 Procter & Gamble Plaza, Cincinnati, OH 45201 (513) 983-1100; Proctor & Gamble Chemicals, 11530 Reed Hartman Highway, Cincinnati, OH 45241, (513) 626-6882; Production site: Sacramento, CA 95828 95828
[SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 602] **PEER REVIEWED**

Sigma-Aldrich Fine Chemicals, 3050 Spruce St., St. Louis MO 63103, (314) 534-4900; Production site: Not specified
[SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 602] **PEER REVIEWED**

Twin Rivers Technologies, 700 Washington St., Quincy, MA 02169, (617) 472-9200; Production site: Quincy, MA 02169
[SRI Consulting. 2007 Directory of Chemical Producers United States. Menlo Park, CA 2007, p. 602] **PEER REVIEWED**

Ecolab Inc., 370 Wabasha St., Ecolab Center, St. Paul MN (Pesticide formulator)
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

West Agro, Inc, 11100 N. Congress Ave., Kansas City MO 64153 (Pesticide formulator)
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

Methods of Manufacturing:

Prepn from octyl bromide; Closson, de Pree, US patent 2,918,494 (1959 to Ethyl Corp). Recovery from Cuphea llavea llave et lex, lythaceae seed oil: Miwa et al, US patent 2,964,546 (1960 to USDA).
[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 2006., p. 285] **PEER REVIEWED**

Fractional distillation of coconut-oil fatty acids
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

Prepared by oxidation of decanol.
[Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 5th ed.Boca Raton, FL 2005, p. 395] **PEER REVIEWED**

General Manufacturing Information:

IDENTIFIED /AS/ COMPONENT OF COFFEE AROMA. /FROM TABLE/
[Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 663] **PEER REVIEWED**

COMPONENT OF BREAD FLAVOR. /FROM TABLE/
[Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 665] **PEER REVIEWED**

CAPRIC ACID COMPOSITION IN RYE CRISPBREAD: 1.0%. /FROM TABLE/
[Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E.

Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 675] **PEER REVIEWED**

USE OF CAPRIC ACID IN PHARMCEUTICAL PREPARATIONS TO IMPROVE RESORPTION PROPERTIES.
[WISCHNIEWSKI M, R HEMPEL; PHARMACEUTICAL PREPARATIONS WITH IMPROVED RESORPTION PROPERTIES; GER OFFEN PATENT NUMBER 2700433 (KALI-CHEMIE PHARMA GMBH) (07/20/78)] **PEER REVIEWED**

FEMA NUMBER 2364
[Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 815] **PEER REVIEWED**

CAPRIC ACID IS USED IN THE PURIFICATION OF WASTEWATERS CONTAINING STARCH.
[SEO Y, J OKADA; JAPAN KOKAI PATENT NUMBER 78 39649 (TOKICO LTD) (04/11/78)] **PEER REVIEWED**

FLAVORS IN WHICH CAPRIC ACID IS USED: BUTTER, COCONUT, FRUIT, LIQUOR, WHISKEY, CHEESE.
[CHEMICALS USED IN FOOD PROCESSING; NAS/NRC PUBL 1274 WASHINGTON DC (1965)] **PEER REVIEWED**

STUDIES INDICATE CAPRIC ACID GLYCEROL MONOCAPRATE HAD STRONG FUNGISTATIC ACTIVITY TOWARDS ASPERGILLUS NIGER, PENICILLUM CITRINUM, CANDIDA UTILIS, & SACCHAROMYCES CEREVISIAE.
[KATO N, SHIBASAKI I; HAKKO KOGAKU ZASSHI 53(11) 793-801 (1975)] **PEER REVIEWED**

Occurs as a glyceride in natural oils.
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

In both the model membrane and guinea pig skin experiments, capric acid is used as an absorption enhancer.
[Miyajima K et al; Chem Pharm Bull 42 (Jun 1994): 1345-7 (1994)] **PEER REVIEWED**

Formulations/Preparations:
Technical; 90%; FCC
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

Grades containing 90 to 100 percent C(10) are available commercially
[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

ECONOSAN ACID SANITIZER: Active Ingredients 8.50% Phosphoric acid; 10.0% Propionic acid; 9.50% Sulfuric acid; 3.00% Capric acid; 3.00% Nonanoic acid
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

MANDATE: Active Ingredients 20.0% Citric acid; 23.8% Phosphoric acid; 6.00% Octanoic acid; 2.00% Capric acid
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

MANDATE PLUS: Active Ingredients 1.09% Capric acid ; 6.30% Nonanoic acid
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

Prifrac 2910 /is/ a mixture of 54% caprylic acid and 44.5% capric (decanoic) acid.
[European Chemicals Bureau; IUCLID Dataset, Decanoic acid (CAS #334-48-5) p.29 (2000 CD-ROM edition). Available from, as of January 21, 2008: http://esis.jrc.ec.europa.eu/ **PEER REVIEWED**

WEST AGRO ACID SANITIZER: Active Ingredient 28.5% Phosphoric acid; 10.0% Propionic acid; 3.00% Capric acid; 3.00% Nonanoic acid
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

Consumption Patterns:

Consumption in the USA for 1980 was 500 tons.
[Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA5 246] **PEER REVIEWED**

U. S. Production:
Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	>1 million - 10 million
1990	>1 million - 10 million
1994	>1 million - 10 million
1998	>10 million - 50 million
2002	>1 million - 10 million

[US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Decanoic Acid (334-48-5). Available from, as of January 14, 2008: http://www.epa.gov/oppt/iur/tools/data/2002-vol.html **PEER REVIEWED**

Decanoic acid is listed as a High Production Volume (HPV) chemical (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).
[EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. Available from the Database Query page at: http://www.epa.gov/hpv/pubs/general/opptsrch.htm on Decanoic Acid (334-48-5) as of February 4, 2008] **PEER REVIEWED**

Laboratory Methods:

Clinical Laboratory Methods:
Analyte: capric acid; matrix: blood (plasma); procedure: high-performance liquid chromatography with fluorescence detection at 365 nm (excitation) and 460 nm (emission); limit of quantitation: 5 pmole
[Tsuchiya H et al; J Chromatogr 309: 43-52 (1984). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: blood (serum); procedure: high-performance liquid chromatography with fluorescence detection at 350 nm (excitation) and 530 nm (emission)
[Yanagisawa I et al; J Chromatogr 345: 229-240 (1985). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: blood (serum); procedure: high-performance liquid chromatography with ultraviolet detection at 400 nm or 230 nm: limit of detection: 0.4-1 pmole (UV 400), 100-200 fmole (UV 230)
[Miwa H et al; J Chromatogr 416: 237-245 (1987). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: blood (serum); procedure: high-performance liquid chromatography with fluorescence detection at 365 nm (excitation) and 447 nm (emission); limit of detection: 1-2 fmole
[Yamaguchi M et al; J Liq Chromatogr 18: 2991-3006 (1995). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: tissue (adipose, blood vessel wall); procedure: high-performance liquid chromatography with ultraviolet detection at 242 nm; limit of detection: 0.8-1.2 ng
[Hanis T et al; J Chromatogr 452: 443-457 (1988). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analytic Laboratory Methods:
THE SIMULATNEOUS GAS CHROMATOGRAPHIC SEPARATION OF A MIXTURE OF 14 LOWER FATTY ACIDS, 11 PHENOLS & 7 INDOLES WAS EFFECTED BY USING A GLASS CAPILLARY COLUMN.

[Y HOSHIKA; J CHROMATOGR 144(2) 181-90 (1977)] **PEER REVIEWED**

Analyte: capric acid; matrix: chemical purity; procedure: gas chromatography with flame ionization detection
[U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p.757 (2007)] **PEER REVIEWED**

Analyte: capric acid; matrix: food (butter, oil, margarine); procedure: high-performance liquid chromatography with fluorescence detection at 365 nm (excitation) and 425 nm (emission) and ultraviolet detection at 252 nm
[Akasaka K et al; Anal Lett 20: 1581-1594 (1987). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: food (fat, oil); procedure: high-performance liquid chromatography with ultraviolet detection at 230 nm; limit of quantitation: 2.5 pmole
[Miwa H, Yamamoto M; J Chromatogr 351: 275-282 (1986). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: food (fat, oil); procedure: high-performance liquid chromatography with ultraviolet detection at 400 nm
[Miwa H, Yamamoto M; J AOAC Int 79: 493-497 (1996). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: food (butter, margarine, orange juice); procedure: high-performance liquid chromatography with ultraviolet detection at 651 nm and with post-column ion-pair extraction and absorbance detection; limit of detection: 39 ng
[Lawrence JF, Charbonneau CF; J Chromatogr 445: 189-197 (1988). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Analyte: capric acid; matrix: food (butter, cheese, condensed milk, ice cream, milk, yogurt); procedure: high-performance liquid chromatography with ultraviolet detection at 400 nm; limit of detection: 0.5-2 pmole
[Miwa H, Yamamoto M; J Chromatogr 523: 235-246 (1990). As cited in: Lunn G; HPLC and CE Methods for Pharmaceutical Analysis. CD-ROM. New York, NY: John Wiley & Sons (2000)] **PEER REVIEWED**

Special References:

Synonyms and Identifiers:

Synonyms:
C-1095
PEER REVIEWED

C10 Fatty acid
PEER REVIEWED

N-CAPRIC ACID
PEER REVIEWED

CAPRINIC ACID
PEER REVIEWED

Caprinsaure
PEER REVIEWED

CAPRYNIC ACID
PEER REVIEWED

CAPRIC ACID
PEER REVIEWED

N-DECANOIC ACID
PEER REVIEWED

Decansaeure
PEER REVIEWED

Decansaeure (Altstoff)
PEER REVIEWED

Decansaure
PEER REVIEWED

DECANsaure (ALTSTOFF)
PEER REVIEWED

Decatoic acid
PEER REVIEWED

N-Decoic acid
PEER REVIEWED

DECOIC ACID
PEER REVIEWED

N-DECOIC ACID
PEER REVIEWED

N-Decylic acid
PEER REVIEWED

DECYLIC ACID
PEER REVIEWED

Docansaure
PEER REVIEWED

Emery 659
PEER REVIEWED

Hexacid 1095
PEER REVIEWED

Lunac 10-95
PEER REVIEWED

NAA 102
PEER REVIEWED

NEO-FAT 10
PEER REVIEWED

1-NONANE CARBOXYLIC ACID
PEER REVIEWED

1-NONANECARBOXYLIC ACID
PEER REVIEWED

Prifac 2906
PEER REVIEWED

Prifac 296
PEER REVIEWED

Prifrac 2906
PEER REVIEWED

USEPA/OPP Pesticide Code: 128955
PEER REVIEWED

Formulations/Preparations:
Technical; 90%; FCC
[Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 227] **PEER REVIEWED**

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[Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 172] **PEER REVIEWED**

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[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

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MANDATE PLUS: Active Ingredients 1.09% Capric acid ; 6.30% Nonanoic acid
[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

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[National Pesticide Information Retrieval System's USEPA/OPP Chemical Ingredients Database on Capric acid (334-48-5). Available from, as of February 6, 2008: http://ppis.ceris.purdue.edu/htbin/epachem.com **PEER REVIEWED**

Administrative Information:

Hazardous Substances Databank Number: 2751

Last Revision Date: 20081007

Last Review Date: Reviewed by SRP 5/8/2008

Update History:
Complete Update on 2008-10-07, 64 fields added/edited/deleted
Complete Update on 05/13/2002, 1 field added/edited/deleted.
Complete Update on 05/15/2001, 1 field added/edited/deleted.
Complete Update on 09/21/1999, 1 field added/edited/deleted.
Complete Update on 08/26/1999, 1 field added/edited/deleted.
Complete Update on 12/15/1997, 50 fields added/edited/deleted.
Field Update on 10/26/1997, 1 field added/edited/deleted.
Complete Update on 10/15/1996, 1 field added/edited/deleted.
Complete Update on 01/24/1996, 1 field added/edited/deleted.
Complete Update on 04/20/1995, 1 field added/edited/deleted.
Complete Update on 04/20/1995, 1 field added/edited/deleted.
Complete Update on 12/28/1994, 1 field added/edited/deleted.
Complete Update on 03/25/1994, 1 field added/edited/deleted.
Field update on 12/26/1992, 1 field added/edited/deleted.
Complete Update on 10/10/1990, 1 field added/edited/deleted.
Complete Update on 04/16/1990, 1 field added/edited/deleted.
Field update on 03/06/1990, 1 field added/edited/deleted.

Complete Update on 11/09/1988, 1 field added/edited/deleted.
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